John please

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

# SEARCH REQUEST FORM

6-717

Requestor's Name: Qazi, Sabeha

Serial Number: 09/214,155

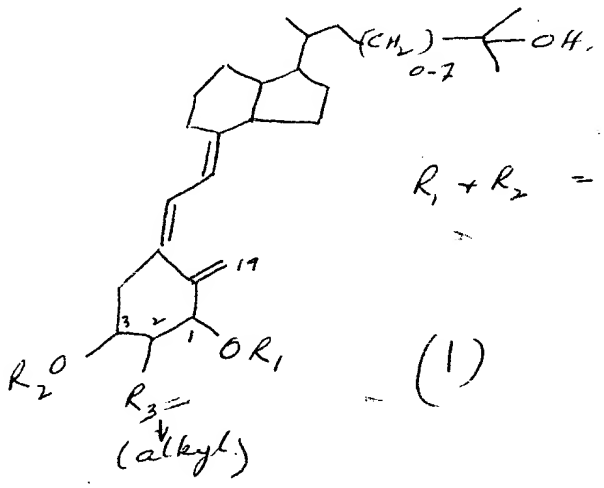
Date: 6/22/99 Phone: 305-3910 Art Unit: 1616 3807

**Search Topic:**

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

Please search for

(1) 1,25-dehydroxy-2-methylvitab-$D_3$ of for(1)

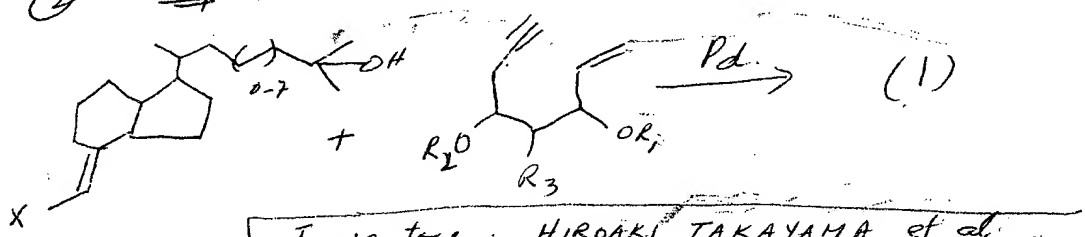



$R_1 + R_2$ = H or Tri (C1-C7 alkyl) silyl gp.

(1)

Point of Contact:
John Dantzman
Technical Info. Specialist
CM1 1E05 Tel: 308-4488

(2) Preparation:-




X = Halogen

(1)

Inventors: HIROAKI TAKAYAMA et al.
Priority. JP 9-114695 5/2/97

## STAFF USE ONLY

Date completed: 6-22-99
Searcher: JOHN D.
Terminal time: 0040
Elapsed time:
CPU time:
Total time: 60
Number of Searches:
Number of Databases:

**Search Site**
- STIC
- ✓ CM-1
- Pre-S

**Type of Search**
- N.A. Sequence
- ✓ A.A. Sequence
- Structure
- Bibliographic

**Vendors**
- ✓ IG
- STN
- Dialog
- APS
- Geninfo
- SDC
- DARC/Questel
- Other

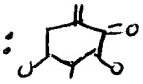
PTO-1590 (9-90)

# SUMMARY



=> d his

(FILE 'REGISTRY' ENTERED AT 14:07:07 ON 22 JUN 1999)
DEL HIS Y
L1 STR
L2 1 S L1
L3 STR L1
L4 1 S L3
L5 36 S L3 FUL ← product + Reactant
L6 STR L3
L7 2 S L5 NOT 46.150.1/RID ← Reactant
L8 34 S L5 NOT L7 ← product

this eliminates : 

FILE 'CAPLUS' ENTERED AT 14:57:26 ON 22 JUN 1999

FILE 'REGISTRY' ENTERED AT 14:57:49 ON 22 JUN 1999

FILE 'CAPLUS' ENTERED AT 14:58:44 ON 22 JUN 1999

FILE 'HCAPLUS' ENTERED AT 15:00:14 ON 22 JUN 1999
L9 11 S L8
L10 9 S L7
L11 4 S L9 AND L10 ← 4 references
SELECT RN L11 1-4

FILE 'REGISTRY' ENTERED AT 15:00:41 ON 22 JUN 1999
L12 109 S E97-205
L13 89 S L12 NOT L5

FILE 'HCAPLUS' ENTERED AT 15:03:36 ON 22 JUN 1999
L14 4 S L9 AND L10 AND L13 ← 4 references plus all compounds in the citations

FILE 'CAOLD' ENTERED AT 15:05:49 ON 22 JUN 1999
L15 0 S L8 AND L7

FILE 'BEILSTEIN' ENTERED AT 15:06:00 ON 22 JUN 1999
L16 STR L3
L17 42 S L16 FUL
L18 STR L16
L19 42 S L18 FUL
L20 STR L18
L21 42 S L20 FUL
L22 42 S L21 AND PRE/FA ← 42 compounds were contained in 4 different References
L23 24 S FUJISHIMA, TOSHIE?/AU AND LIU, ZHAOPENG?/AU AND MIURA, DAISHI
L24 26 S L22 NOT L23
L25 98 S KONNO, KATSUHIRO?/AU AND MAKI, SHOJIRO?/AU AND FUJISHIMA, TOS
L26 98 S L25 AND 1998/PY
L27 10 S L24 NOT L26
L28 25 S ONO, YOSHIYUKI?/AU AND WATANABE, HIROYOSHI?/AU AND SHIRAISHI,
L29 25 S L28 AND 1997/PY
L30 5 S L27 NOT L29
L31 55 S POSNER, GARY H?/AU AND CHO, CHEON-GYU?/AU AND ANJEH, TIZAH E.
L32 55 S L31 AND 1995/PY
L33 0 S L30 NOT L32

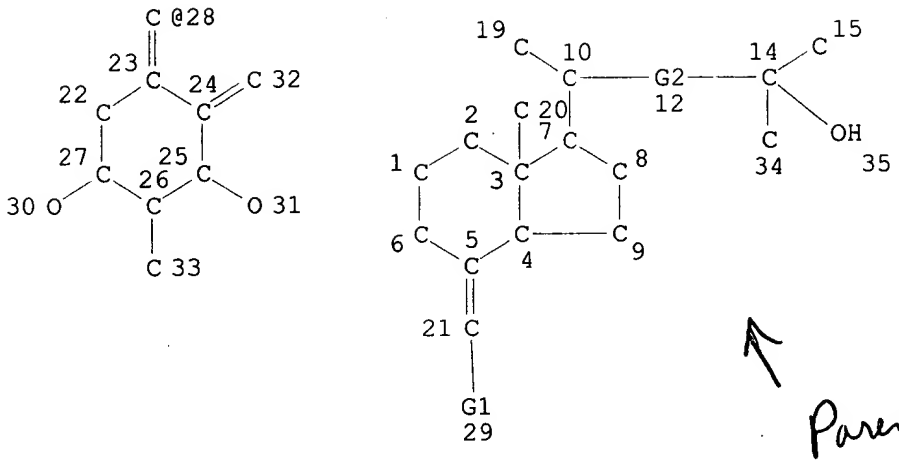
I printed 4 references.

FILE 'USPATFULL' ENTERED AT 15:15:15 ON 22 JUN 1999
L34 1 S L8
L35 0 S L34 AND L7 ← ∅ hits USPat file

FILE 'CASREACT' ENTERED AT 15:15:37 ON 22 JUN 1999
L36 3 S L8
L37 5 S L7
L38 1 S L36 AND L37 ← 1 reaction Casreact

=> d que l7

L3 STR



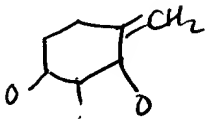

Parent Search covers Product and reactant.

VAR G1=X/28
REP G2=(0-9) CH2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

This get rid of




L5 36 SEA FILE=REGISTRY SSS FUL L3
L7 2 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT 46.150.1/RID

Reactant.

=> d bib abs hitstr

L14 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 1999 ACS
AN 1999:271054 HCAPLUS
DN 130:296894
TI Preparation of vitamin D3 derivatives for the treatment of osteoporosis
IN Takayama, Hiroaki; Konno, Katsuhiro; Maki, Shojiro
PA Teijin Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | JP 11116551 | A2 | 19990427 | JP 98-160647 | 19970502 |
| PRAI | JP 96-235144 | 19960905 | | | |
| | JP 96-314693 | 19961126 | | | |
| | JP 97-114695 | 19970502 | | | |

OS MARPAT 130:296894
GI

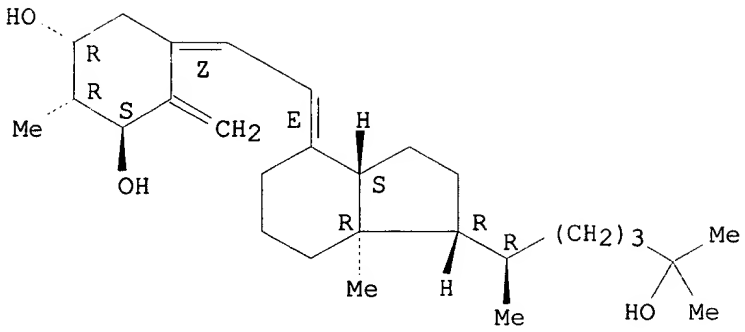
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-methylvitamin D3 derivs. of formula I [R1, R2 = H, alkyl]
are prepd. for the treatment of osteoporosis. Thus, III was added to IV, then deprotected to give II. The vitamin D receptor affinity of II was 400, compared to 100 for 1.alpha.,25-dihydroxyvitamin D3.

IT **158388-11-5P 203126-73-2P 203126-91-4P**
**203126-92-5P 203126-93-6P 203126-94-7P**
**203126-95-8P 203126-96-9P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)

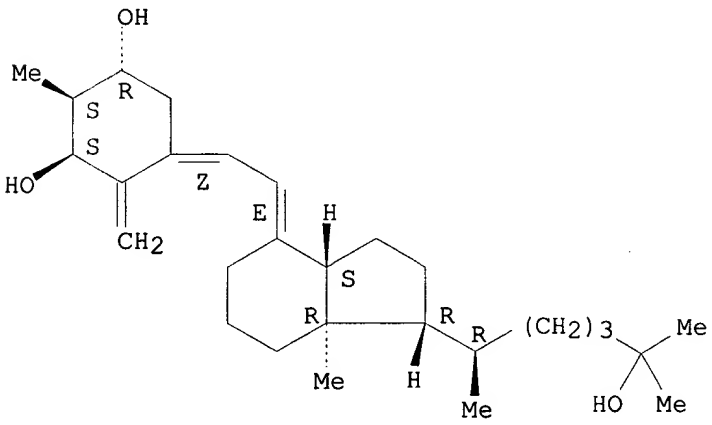
RN 158388-11-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



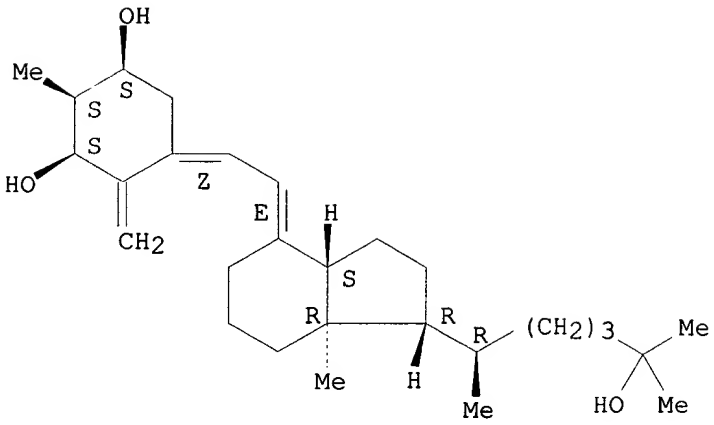
RN 203126-73-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



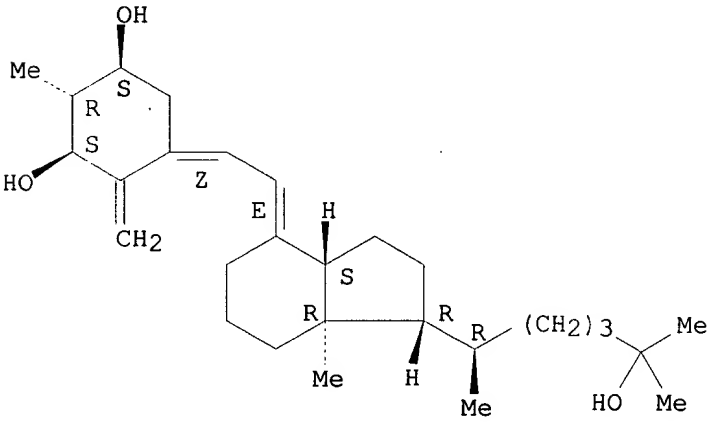
RN 203126-91-4 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



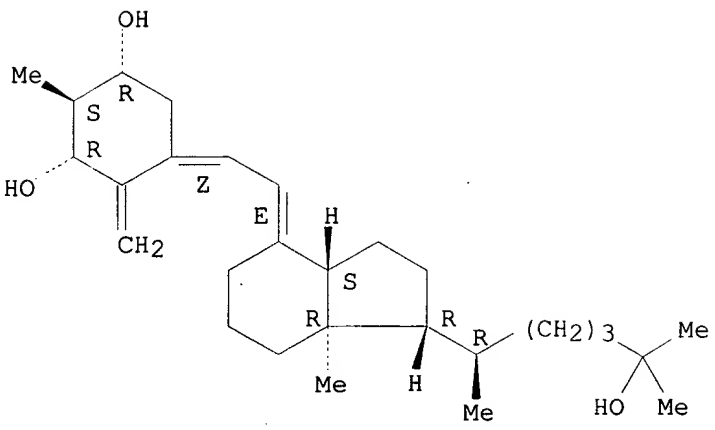
RN 203126-92-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



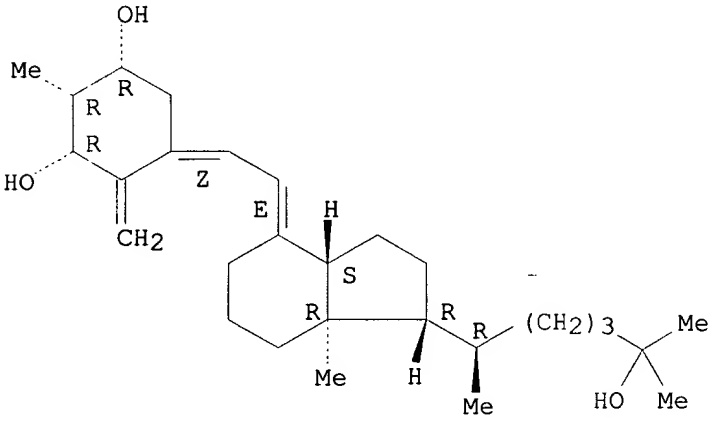
RN 203126-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



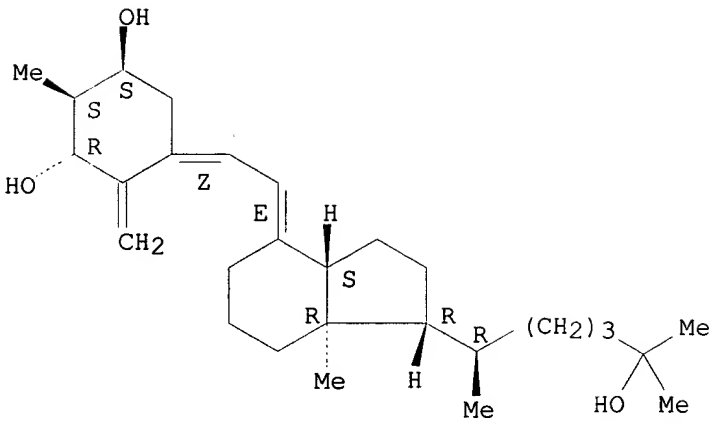
RN 203126-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



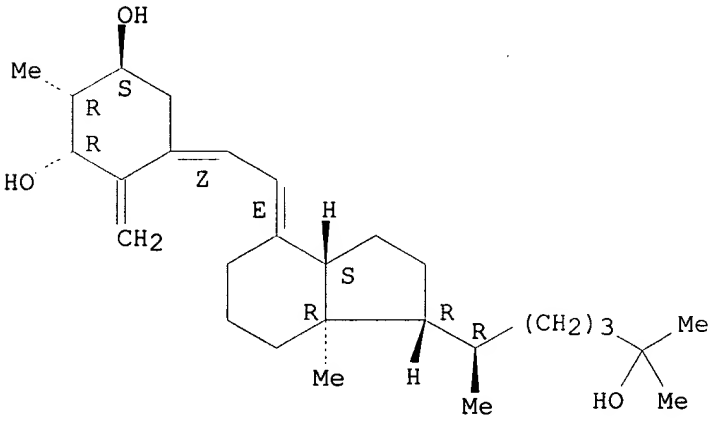
RN 203126-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 203126-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

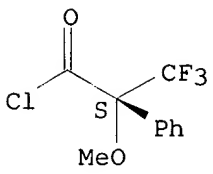


IT **1066-54-2**, Ethynyltrimethylsilane **20445-33-4**, (S)-MTPA-Cl **39637-99-5**, (R)-MTPA-Cl **80657-57-4** **143705-63-9**
RL: RCT (Reactant)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)
RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$Me_3Si-C\equiv CH$

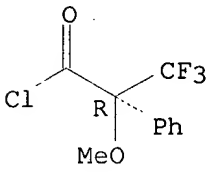
RN 20445-33-4 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



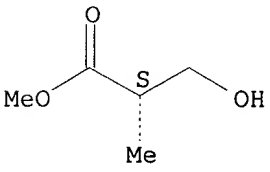
RN 39637-99-5 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



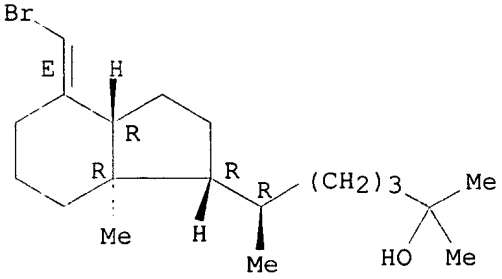
RN 80657-57-4 HCAPLUS
CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 143705-63-9 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

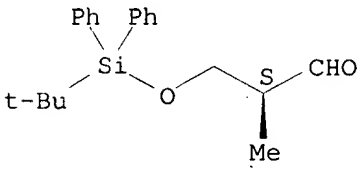


IT **92817-88-4P 95514-03-7P 95514-04-8P 132117-93-2P 203126-90-3P 215394-09-5P**

**215394-10-8P 215394-12-0P 215394-15-3P**
**215394-17-5P 215394-20-0P 215394-22-2P**
**215394-23-3P 215394-24-4P 215394-34-6P**
**215394-35-7P 215394-36-8P 223437-33-0P**
**223437-37-4P 223437-39-6P 223437-51-2P**
**223437-60-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)

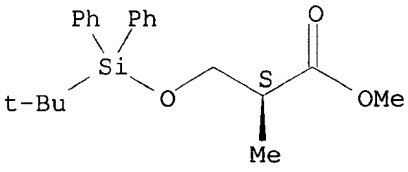
RN 92817-88-4 HCAPLUS
CN Propanal, 3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



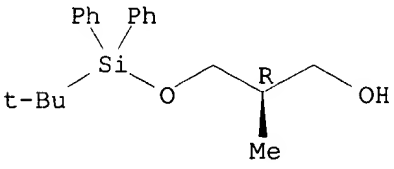

RN 95514-03-7 HCAPLUS
CN Propanoic acid, 3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



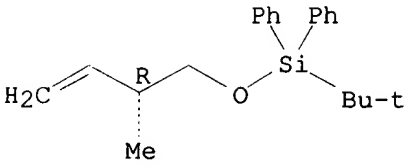

RN 95514-04-8 HCAPLUS
CN 1-Propanol, 3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-, (2R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



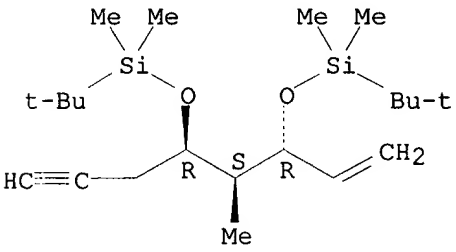

RN 132117-93-2 HCAPLUS
CN Silane, (1,1-dimethylethyl)[[(2R)-2-methyl-3-butenyl]oxy]diphenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



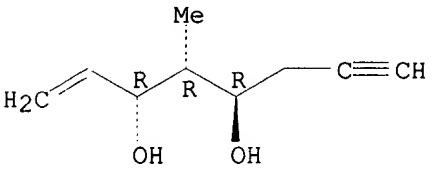
RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



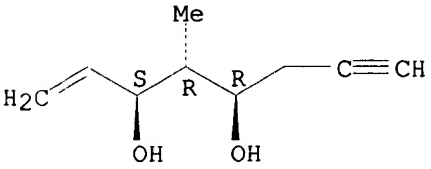
RN 215394-09-5 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



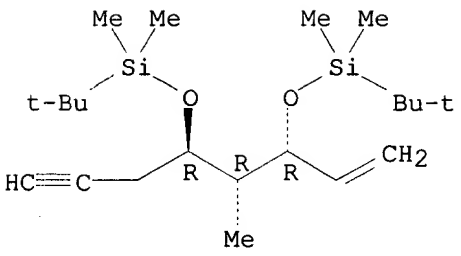
RN 215394-10-8 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3S,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



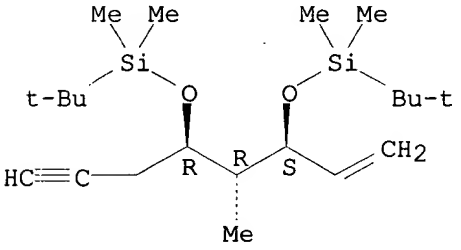
RN 215394-12-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



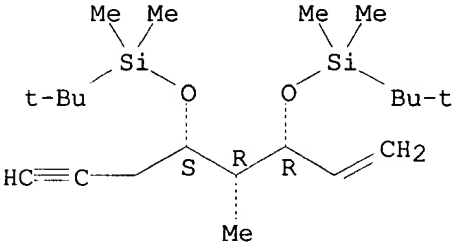
RN 215394-15-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



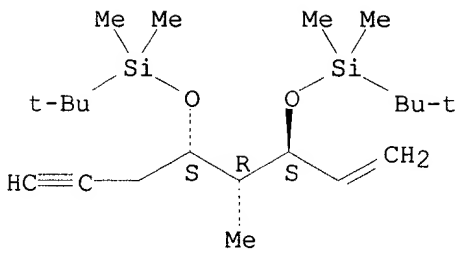
RN 215394-17-5 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



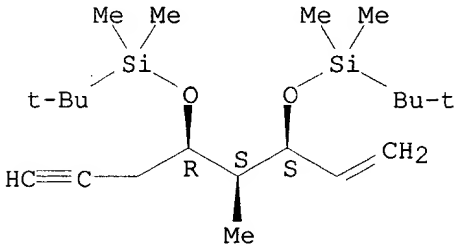
RN 215394-20-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



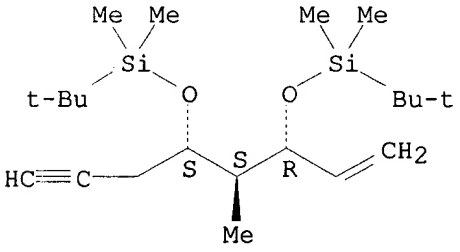
RN 215394-22-2 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



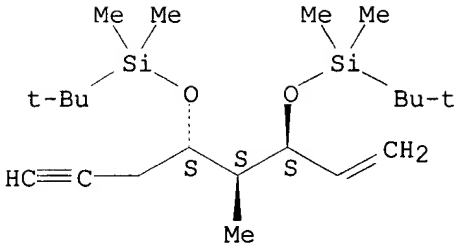
RN 215394-23-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



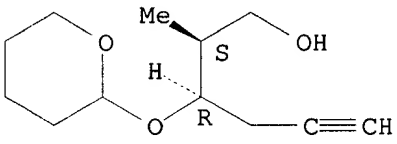
RN 215394-24-4 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



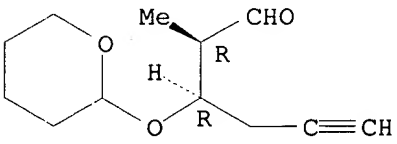
RN 215394-34-6 HCAPLUS
CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



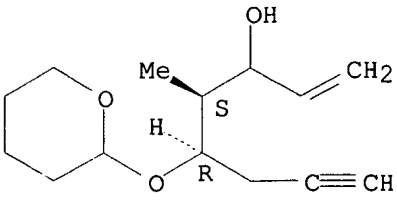
RN 215394-35-7 HCAPLUS
CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



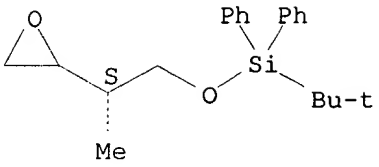
RN 215394-36-8 HCAPLUS
CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



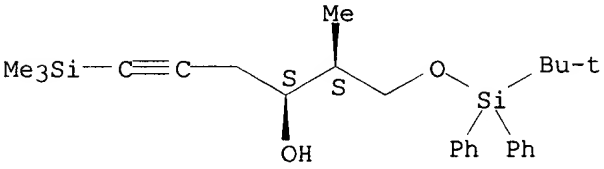
RN 223437-33-0 HCAPLUS
CN Silane, (1,1-dimethylethyl)[(2S)-2-oxiranylpropoxy]diphenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



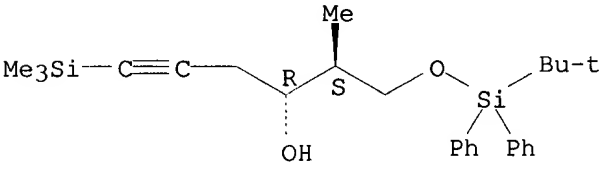
RN 223437-37-4 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



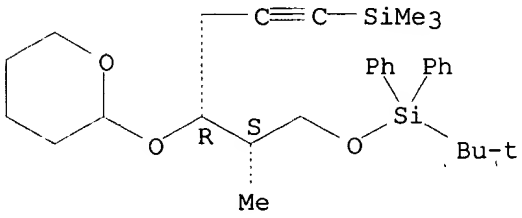
RN 223437-39-6 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



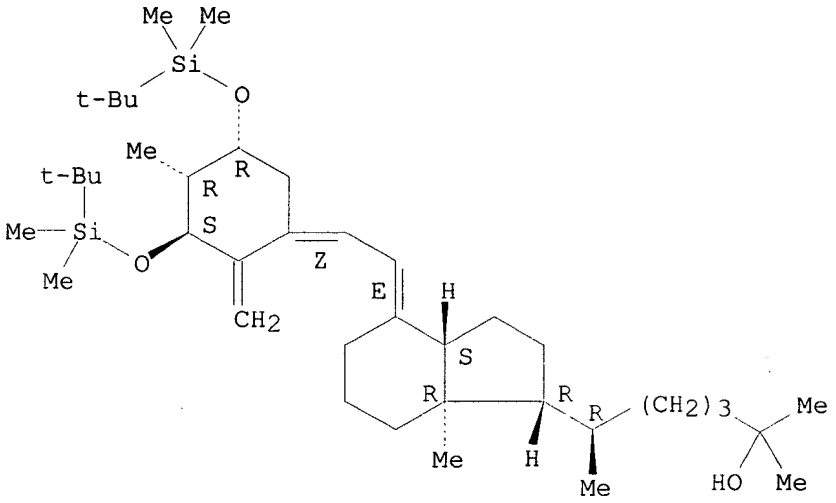
RN 223437-51-2 HCAPLUS
CN Silane, [(4R,5S)-6-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-5-methyl-4-[(tetrahydro-2H-pyran-2-yl)oxy]-1-hexynyl]trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



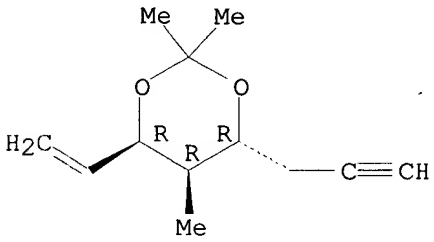
RN 223437-60-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-trien-25-ol, 1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7
E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



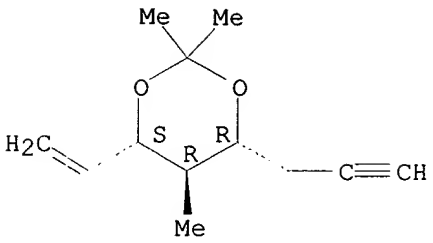
IT **215394-37-9P 215394-38-0P 223437-41-0P**
**223437-43-2P 223437-46-5P 223437-49-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)
RN 215394-37-9 HCAPLUS
CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4R,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



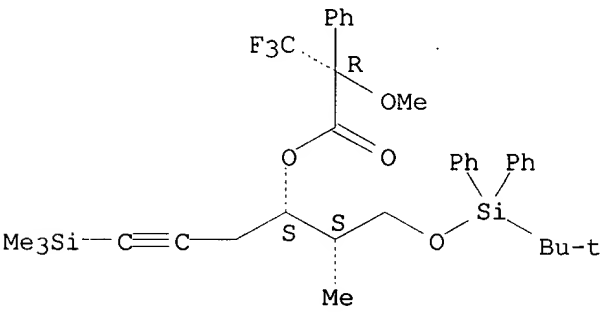
RN 215394-38-0 HCAPLUS
CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4S,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



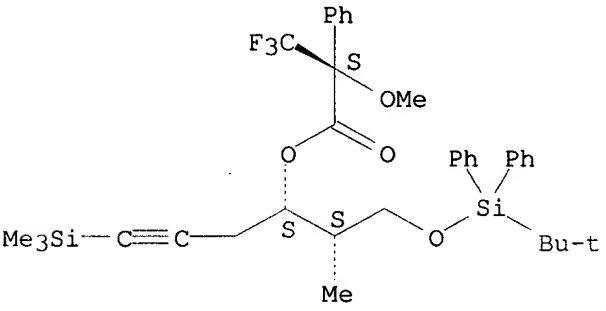
RN 223437-41-0 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



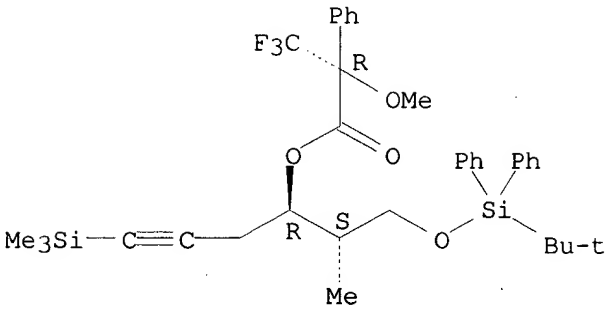
RN 223437-43-2 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



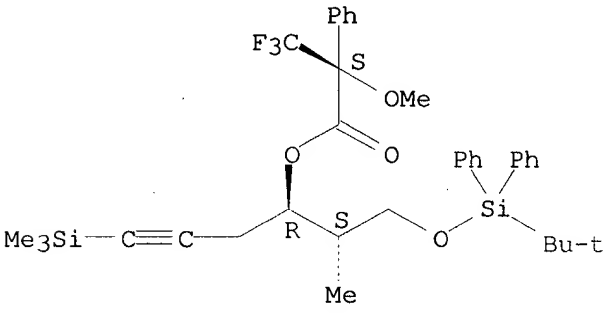
RN 223437-46-5 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 223437-49-8 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d bib abs hitstr 2

L14 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:745027 HCAPLUS
DN 129:343629
TI Preparation of vitamin D3 derivatives and their pharmaceutical uses
IN Takayama, Hiroaki; Konno, Katsuhiro; Fujishima, Toshie
PA Teijin Ltd., Japan
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9850353 | A1 | 19981112 | WO 98-JP1979 | 19980430 |
| | W: JP, US | | | | |
| | RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| PRAI | JP 97-114695 | | 19970502 | | |

OS CASREACT 129:343629; MARPAT 129:343629
GI

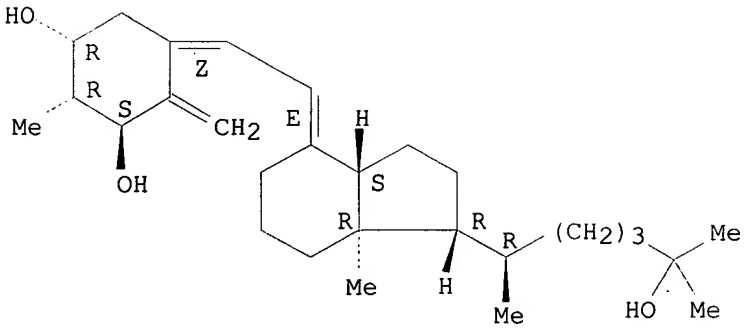
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-Me vitamin D3 derivs. I [R1, R2 = H, tri(C1-7alkyl)silyl; the asym. carbon atoms at the 1-, 2- and 3-positions each independently has an .alpha.- or .beta.-configuration], useful as remedies for osteoporosis, rachitis, accessory thyroidal hyperenergia, etc., are prepd. via reaction of II (X = bromo, iodo) with III (R3, R4 = H, trihydrocarbylsilyl) in the presence of a palladium catalyst optionally followed by deprotection (removal of silyl groups). Thus, II (X = Br) was reacted with III (R3 = R4 = TBS) in toluene contg. Et3N, Pd2(dba)3.CHCl3, and Ph3P at 120.degree. to give IV (R = TBS), which was treated with camphor-10-sulfonic acid in methanol to give 63% IV (R = H). In a study using 1.alpha.,25-dihydroxyvitamin D3 receptors in the bovine thymus gland, this showed an affinity of 160 compared with 100 for 1.alpha.,25-dihydroxyvitamin D3.

IT **158388-11-5P 214351-93-6P 214351-94-7P**
**214351-95-8P 214351-96-9P 214351-97-0P**
**214351-98-1P 214351-99-2P 215394-65-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)

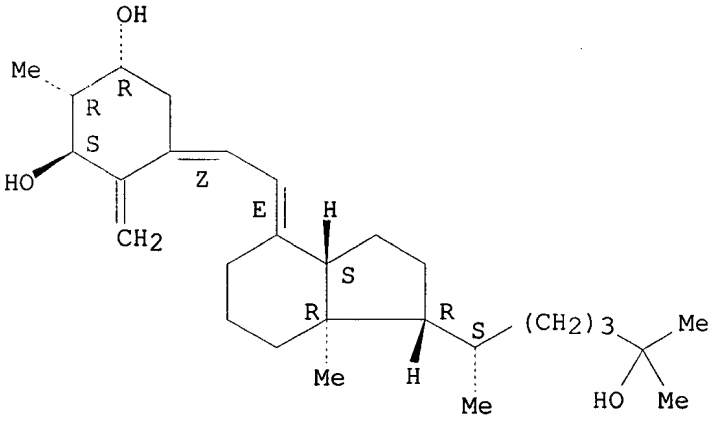
RN 158388-11-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



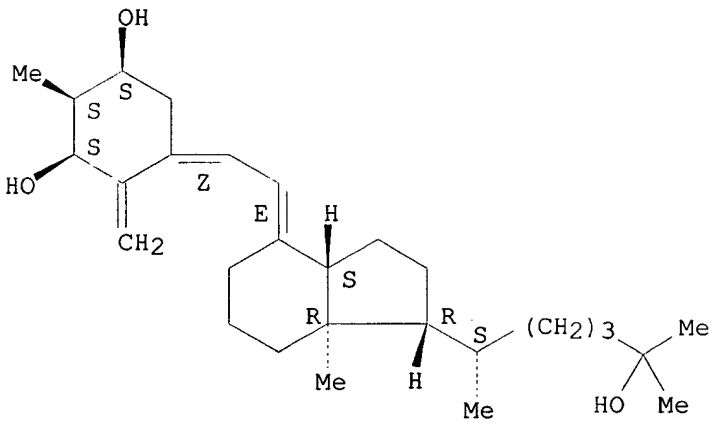
RN 214351-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



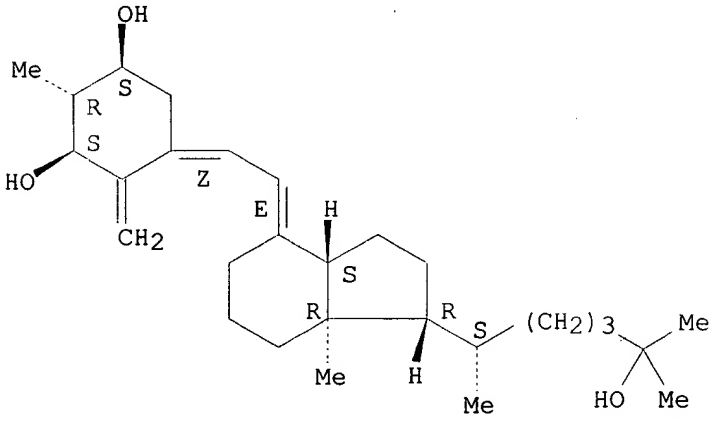
RN 214351-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



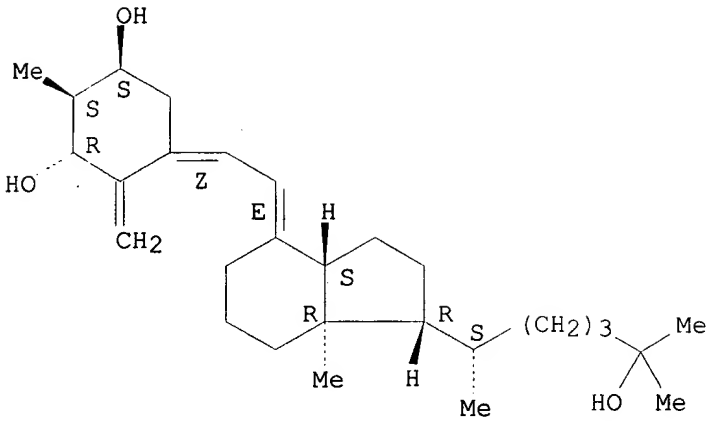
RN 214351-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



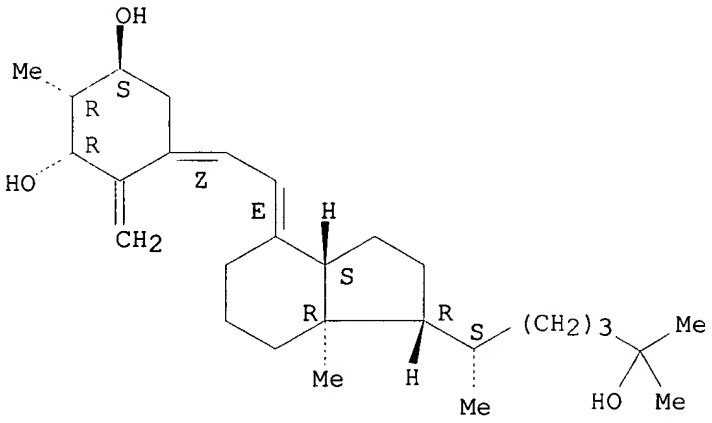
RN 214351-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



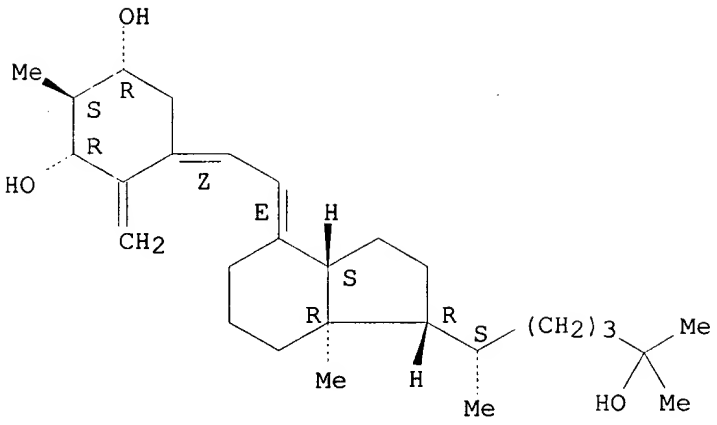
RN 214351-97-0 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



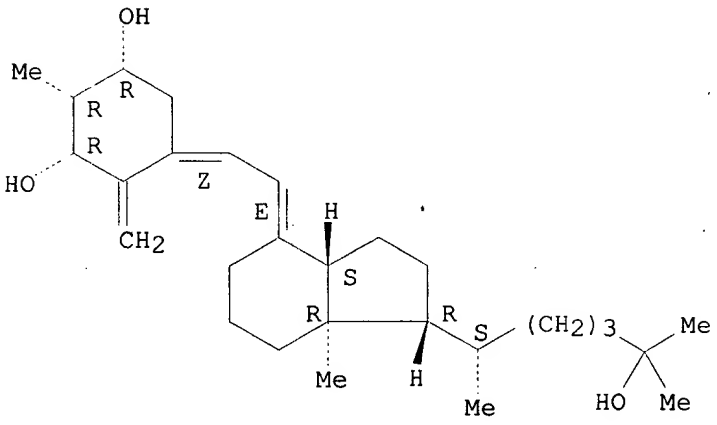
RN 214351-98-1 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



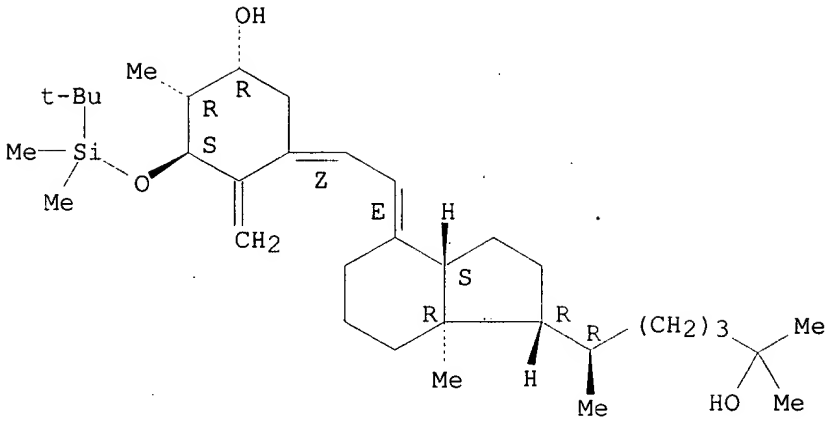
RN 214351-99-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 215394-65-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-3,25-triol, 1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

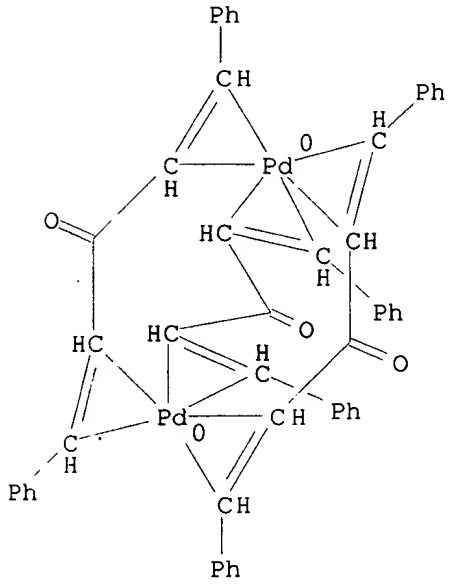
Absolute stereochemistry.
Double bond geometry as shown.



IT **52522-40-4**
RL: CAT (Catalyst use); USES (Uses)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 52522-40-4 HCAPLUS
CN Palladium, tris[.mu.-[(1,2-.eta.:4,5-.eta.)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]di-, compd. with trichloromethane (1:1) (9CI) (CA INDEX NAME)

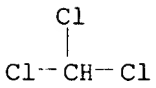
CM 1

CRN 51364-51-3
CMF C51 H42 O3 Pd2
CCI CCS
CDES 2:ALL,E

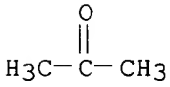


CM 2

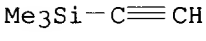
CRN 67-66-3
CMF C H Cl3



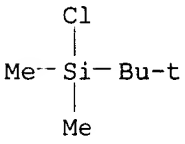
IT **67-64-1**, 2-Propanone, reactions **1066-54-2**, Ethynyltrimethylsilane **18162-48-6**, tert-Butyldimethylsilyl chloride **20445-33-4 39637-99-5 69739-34-0**, tert-Butyldimethylsilyl triflate **143705-63-9 214351-89-0**
RL: RCT (Reactant)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

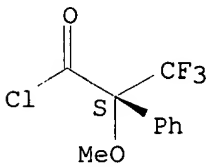


RN 18162-48-6 HCAPLUS
CN Silane, chloro(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 20445-33-4 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (.alpha.S)- (9CI) (CA INDEX NAME)

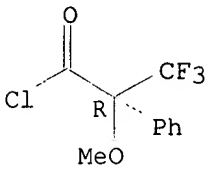
Absolute stereochemistry. Rotation (+).



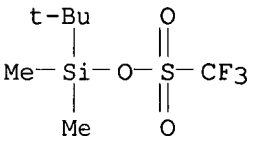
RN 39637-99-5 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,

(.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

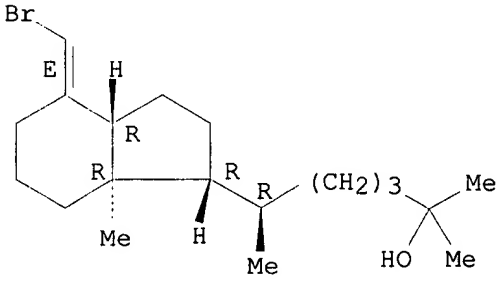


RN 69739-34-0 HCAPLUS
CN Methanesulfonic acid, trifluoro-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)



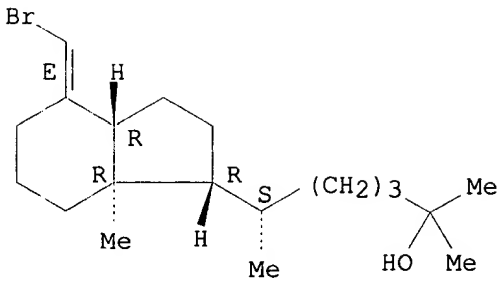
RN 143705-63-9 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-
. .alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-89-0 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-
.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

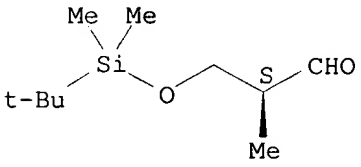
Absolute stereochemistry.
Double bond geometry as shown.




IT **104701-87-3P 112057-64-4P 147915-53-5P**
**147915-54-6P 203126-90-3P 215394-09-5P**
**215394-10-8P 215394-12-0P 215394-15-3P**
**215394-17-5P 215394-20-0P 215394-22-2P**
**215394-23-3P 215394-24-4P 215394-25-5P**
**215394-26-6P 215394-27-7P 215394-28-8P**
**215394-29-9P 215394-30-2P 215394-31-3P**
**215394-32-4P 215394-33-5P 215394-34-6P**
**215394-35-7P 215394-36-8P 215394-37-9P**
**215394-38-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)

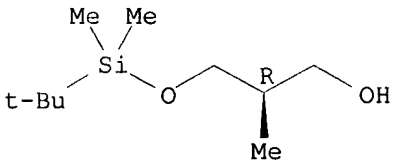
RN 104701-87-3 HCAPLUS
CN Propanal, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.



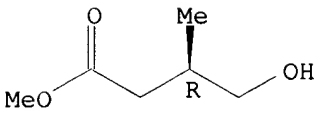

RN 112057-64-4 HCAPLUS
CN 1-Propanol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



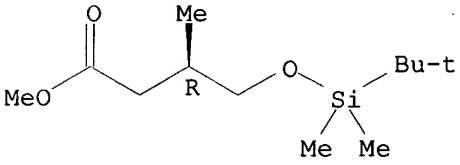

RN 147915-53-5 HCAPLUS
CN Butanoic acid, 4-hydroxy-3-methyl-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



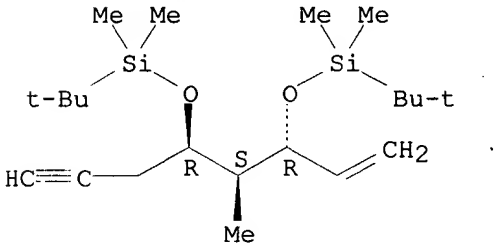
RN 147915-54-6 HCAPLUS
CN Butanoic acid, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methyl-, methyl
ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



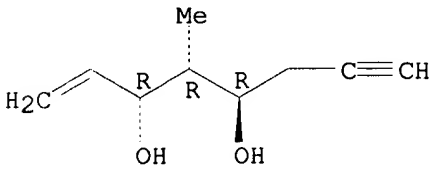
RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



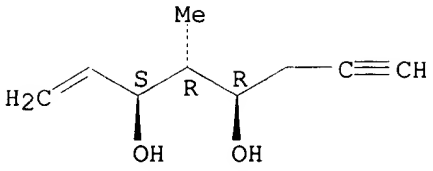
RN 215394-09-5 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



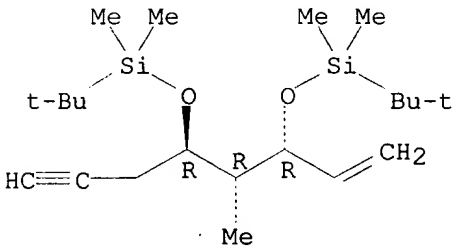
RN 215394-10-8 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3S,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



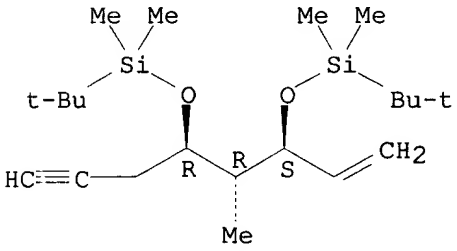
RN 215394-12-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



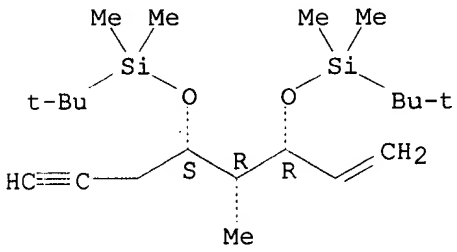
RN 215394-15-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



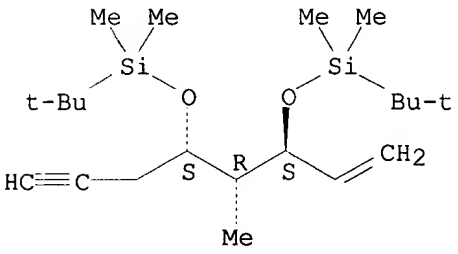
RN 215394-17-5 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



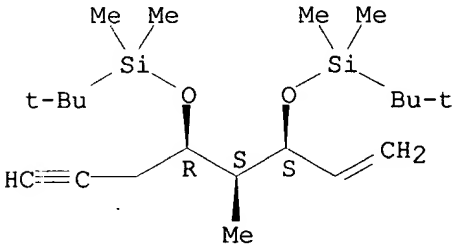
RN 215394-20-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



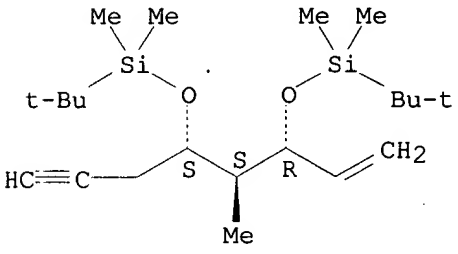

RN 215394-22-2 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



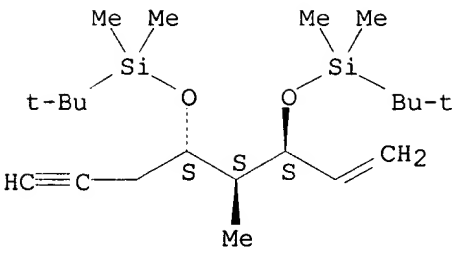

RN 215394-23-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



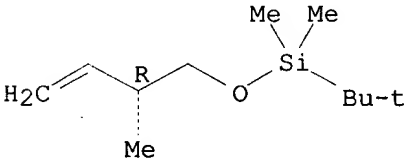

RN 215394-24-4 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



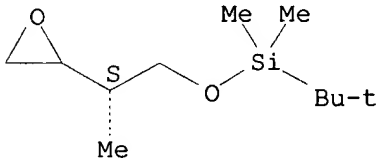
RN 215394-25-5 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(2R)-2-methyl-3-butenyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



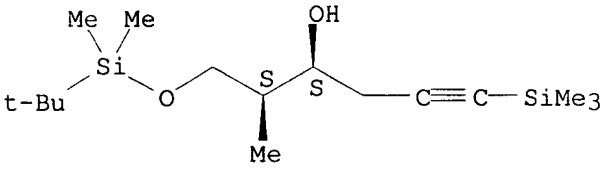
RN 215394-26-6 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[(2S)-2-oxiranylpropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



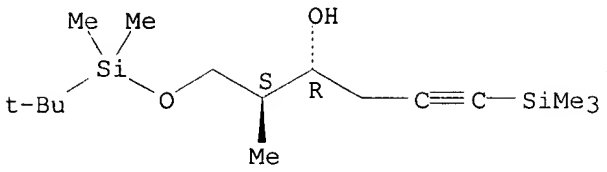
RN 215394-27-7 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



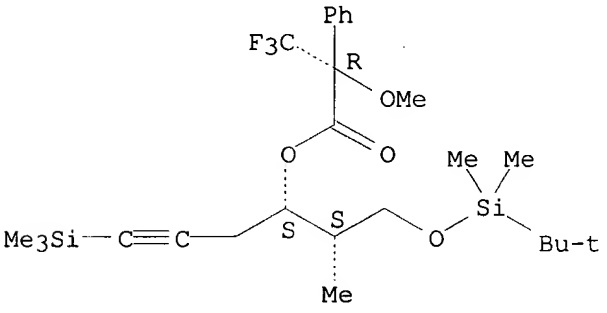
RN 215394-28-8 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



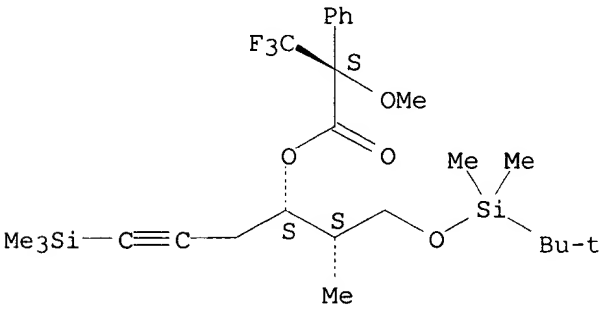
RN 215394-29-9 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



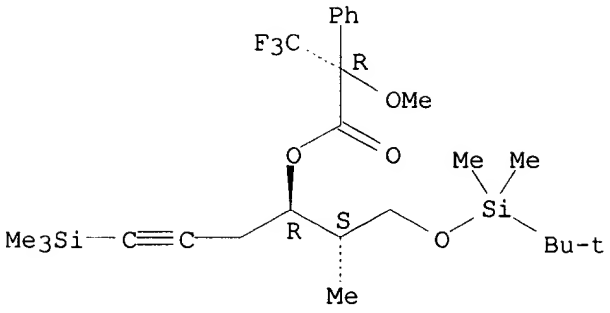
RN 215394-30-2 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



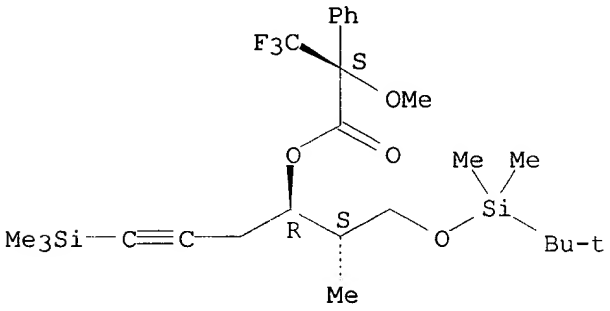
RN 215394-31-3 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



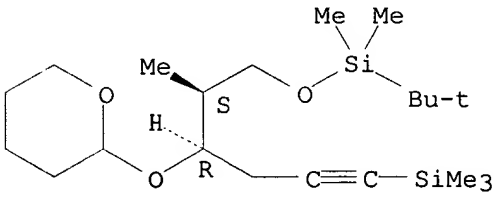
RN 215394-32-4 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



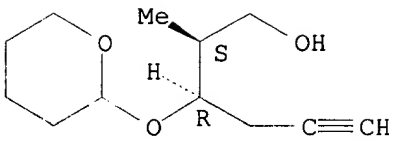
RN 215394-33-5 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[(2S,3R)-2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-3-[3-(trimethylsilyl)-2-propynyl]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



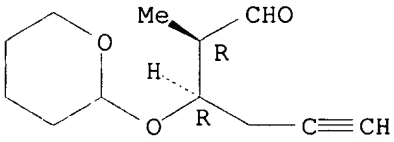
RN 215394-34-6 HCAPLUS
CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



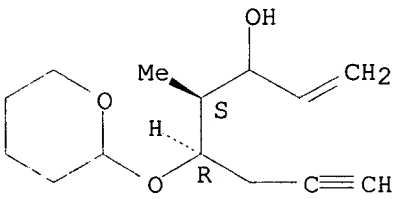

RN 215394-35-7 HCAPLUS
CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



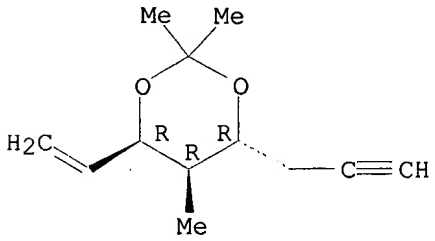

RN 215394-36-8 HCAPLUS
CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



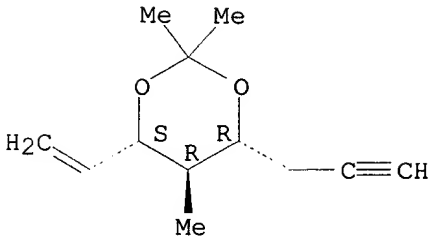

RN 215394-37-9 HCAPLUS
CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4R,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 215394-38-0 HCAPLUS
CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4S,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


Me
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R
H2C
C≡CH
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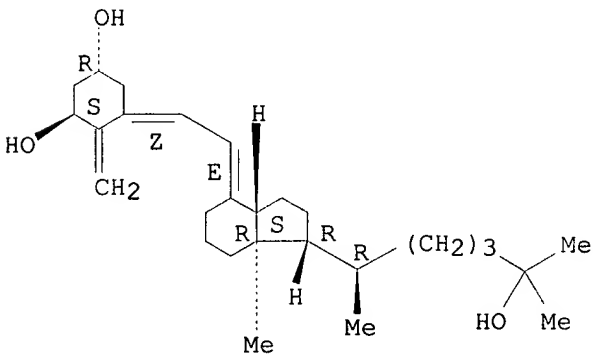
L14 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:606883 HCAPLUS
DN 129:290279
TI Synthesis and biological activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3
AU Fujishima, Toshie; Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Ishizuka, Seiichi; Konno, Katsuhiro; Takayama, Hiroaki
CS Faculty of Pharmaceutical Sciences, Teikyo University, Kanagawa, 199-0195, Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(16), 2145-2148
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB Synthesis and biol. evaluation of all eight possible A-ring diastereomers of 2-methyl-20-epi-1,25-dihydroxyvitamin D3 are described. Among the analogs synthesized, 2.alpha.-methyl-20-epi-1.alpha.,25-dihydroxyvitamin D3 exhibited exceptionally high potency. The double modification of 2-Me substitution and 20-epimerization yielded analogs with unique activity profiles.
IT **32222-06-3P**, 1.alpha.,25-Dihydroxyvitamin D3
RL: PNU (Preparation, unclassified); PREP (Preparation)
(Synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)
RN 32222-06-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

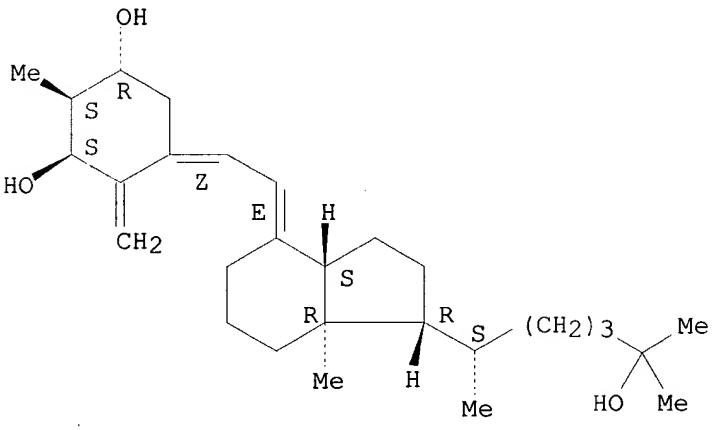
Absolute stereochemistry.
Double bond geometry as shown.




IT **214351-84-5P 214351-93-6P 214351-94-7P**
**214351-95-8P 214351-96-9P 214351-97-0P**
**214351-98-1P 214351-99-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)

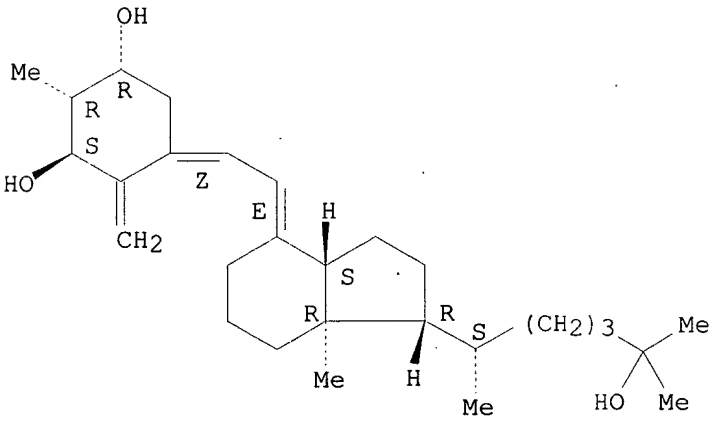
RN 214351-84-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



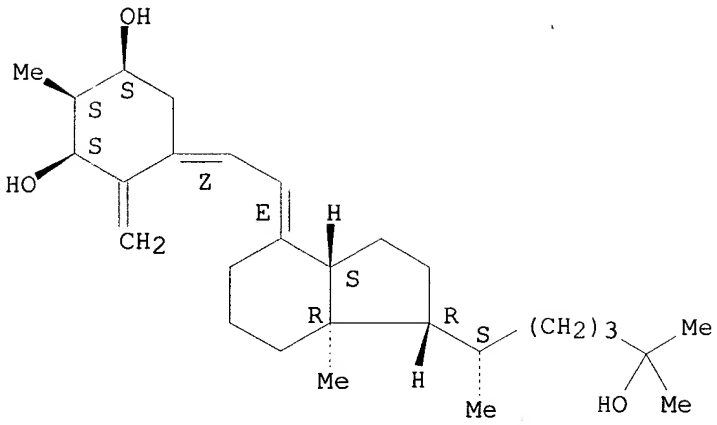
RN 214351-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



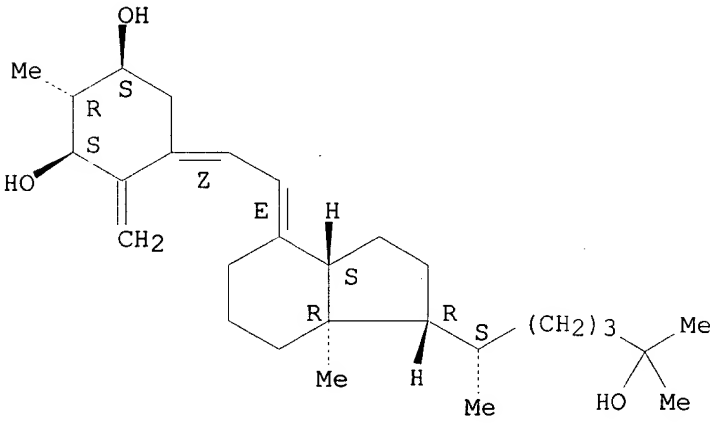
RN 214351-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



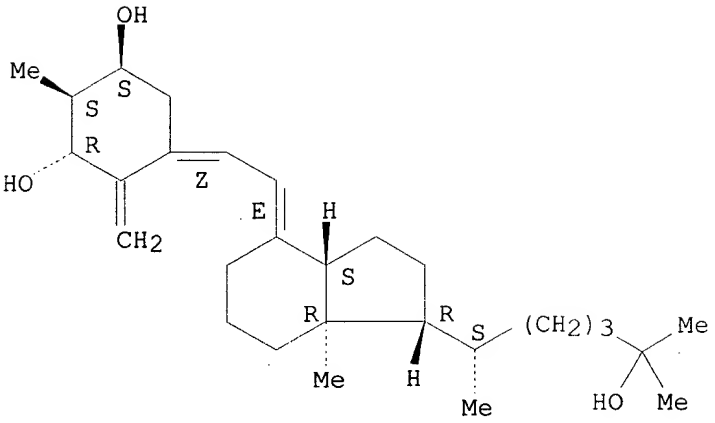
RN 214351-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



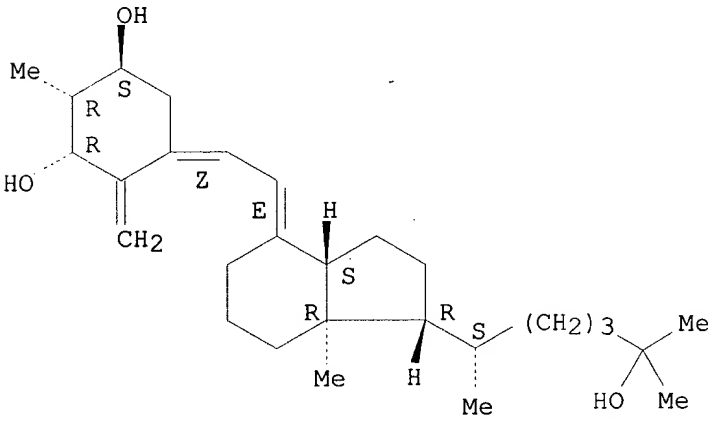
RN 214351-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



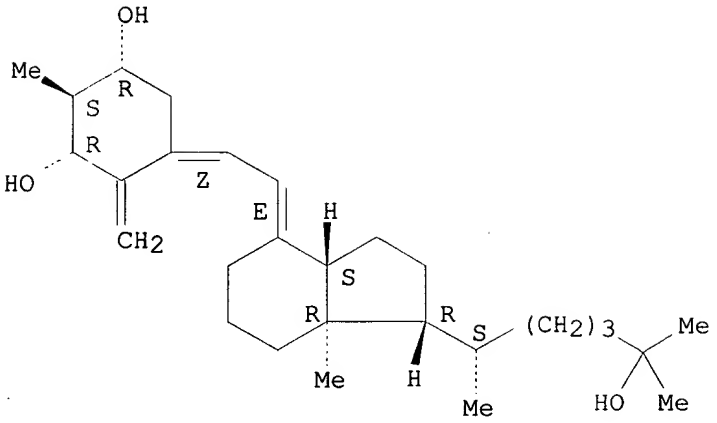

RN 214351-97-0 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



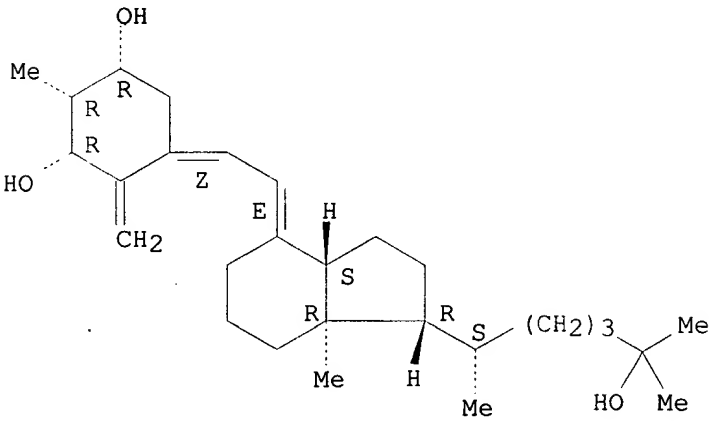

RN 214351-98-1 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



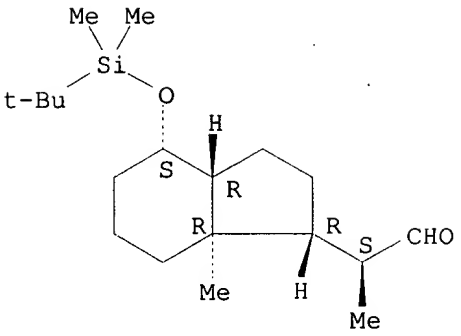
RN 214351-99-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



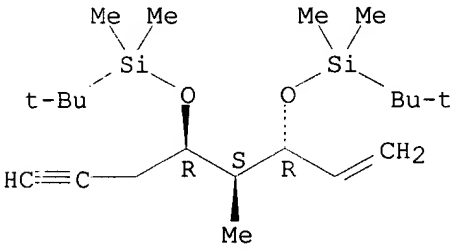
IT **104651-47-0 203126-90-3 214351-87-8**
RL: RCT (Reactant)
(synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)
RN 104651-47-0 HCAPLUS
CN 1H-Indene-1-acetaldehyde, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.alpha.,7a-dimethyl-, (.alpha.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

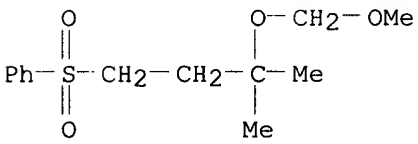


RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

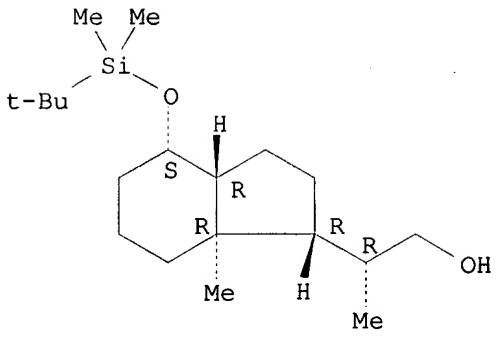


RN 214351-87-8 HCAPLUS
CN Benzene, [[3-(methoxymethoxy)-3-methylbutyl]sulfonyl]- (9CI) (CA INDEX NAME)



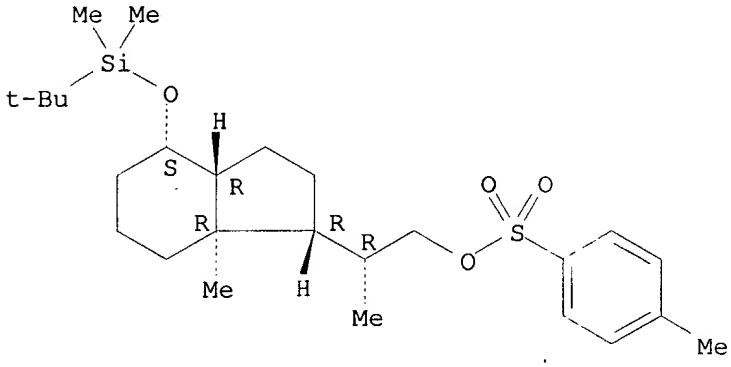
IT **171011-48-6P 183506-75-4P 213250-67-0P**
**214351-86-7P 214351-88-9P 214351-89-0P**
**214351-91-4P 214351-92-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)
RN 171011-48-6 HCAPLUS
CN 1H-Indene-1-ethanol, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, (.beta.R,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



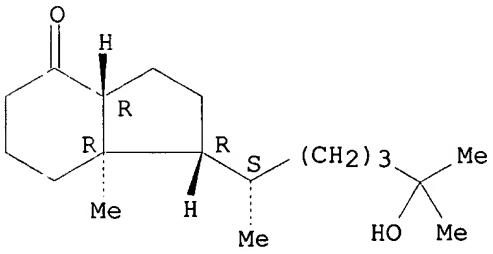
RN 183506-75-4 HCAPLUS
CN 1H-Indene-1-ethanol, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, 4-methylbenzenesulfonate, (.beta.R,1R,3aR,4S,7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



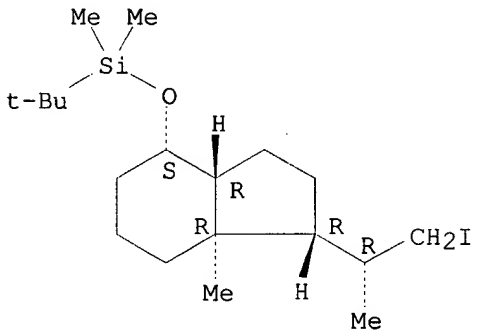
RN 213250-67-0 HCAPLUS
CN 4H-Inden-4-one,
octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-,
(1R,3aR,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



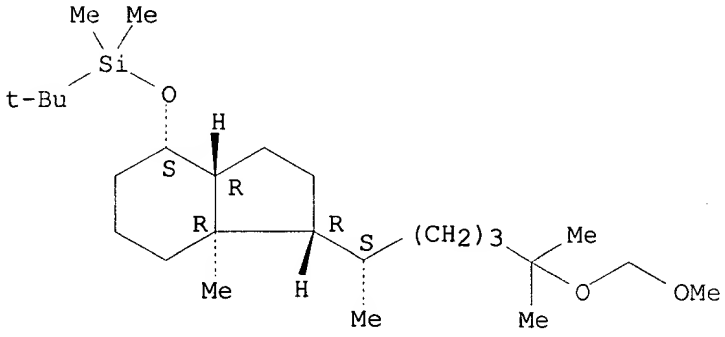
RN 214351-86-7 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-2-iodo-1-methylethyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



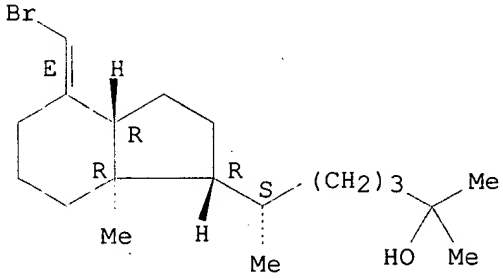
RN 214351-88-9 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1S)-5-(methoxymethoxy)-1,5-dimethylhexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214351-89-0 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)-(9CI) (CA INDEX NAME)

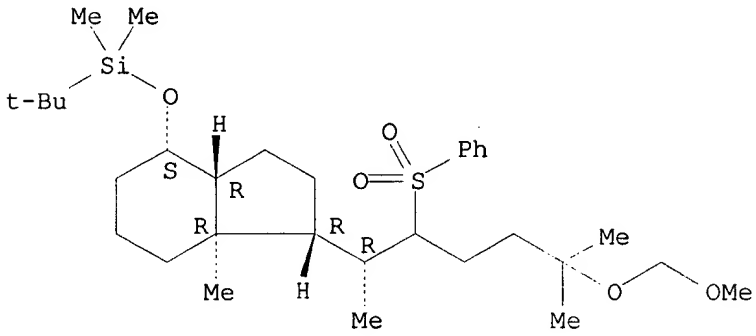
Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-91-4 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-5-

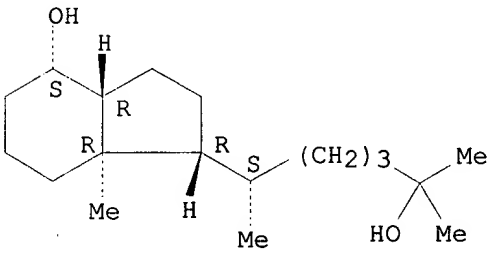
(methoxymethoxy)-1,5-dimethyl-2-(phenylsulfonyl)hexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



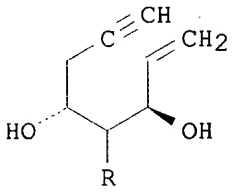

RN 214351-92-5 HCAPLUS
CN 1H-Indene-1-pentanol, octahydro-4-hydroxy-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d bib abs hitstr 4

L14 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:85846 HCAPLUS
DN 128:180577
TI A novel and practical route to A-ring enyne synthon for 1.alpha.,25-dihydroxyvitamin D3 analogs: synthesis of A-ring diastereomers of 1.alpha.,25-dihydroxyvitamin D3 and 2-methyl-1,25-dihydroxyvitamin D3
AU Konno, Katsuhiro; Maki, Shojiro; Fujishima, Toshie; Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Takayama, Hiroaki
CS Faculty Pharmaceutical Sciences, Teikyo Univ., Sagamiko, Kanagawa, 199-01, Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(2), 151-156
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 128:180577
GI

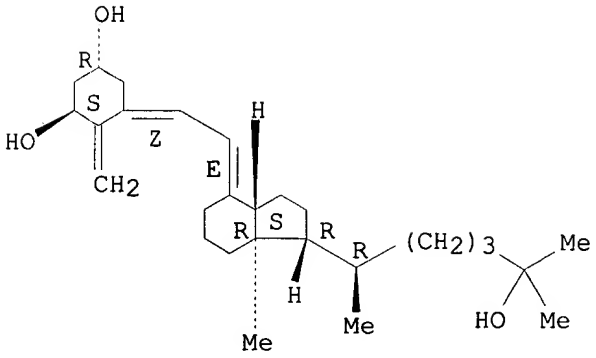



II

AB A novel and practical route to the A-ring enyne synthon II (R = H, Me), which can be versatile for a variety of A-ring analogs of 1.alpha.,25-dihydroxyvitamin D3 (I), was developed. This novel method led to an improved synthesis of the A-ring diastereomers of I, and synthesis of the new analogs, 2-methyl-1,25-dihydroxyvitamin D3 with its all possible diastereomers. The biol. evaluation of the 2-Me analogs showed the .alpha..alpha..beta.-isomer to be more potent than I.

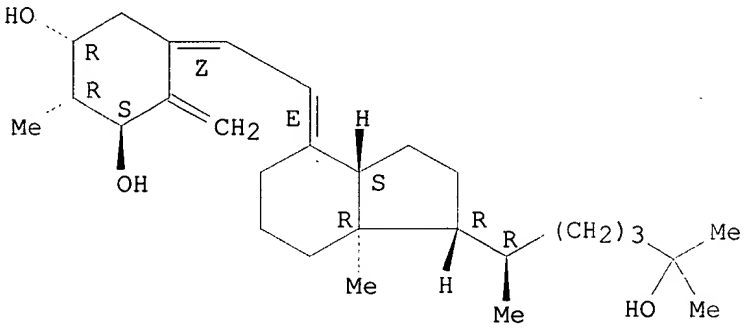
IT **32222-06-3DP**, 1.alpha.,25-Dihydroxyvitamin D3, A-ring analogs **158388-11-5P 203126-73-2P 203126-91-4P 203126-92-5P 203126-93-6P 203126-94-7P 203126-95-8P 203126-96-9P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)
RN 32222-06-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



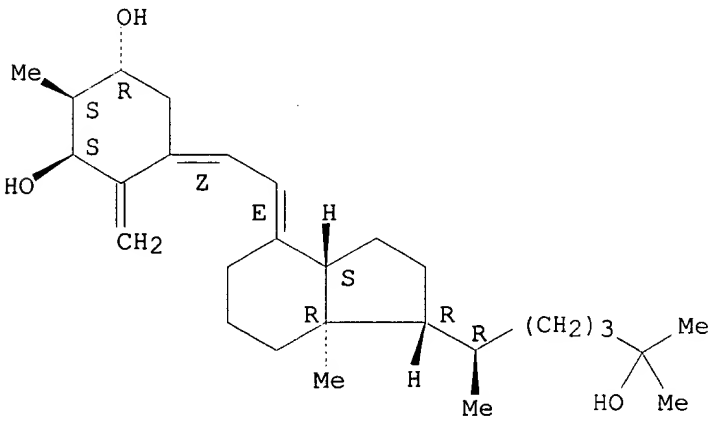
RN 158388-11-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



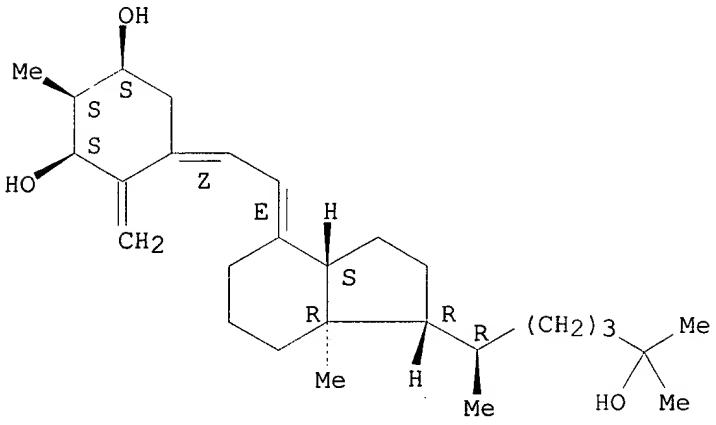
RN 203126-73-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



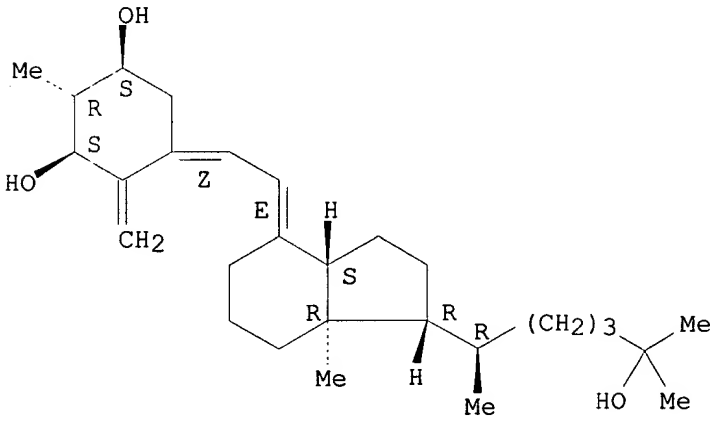
RN 203126-91-4 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



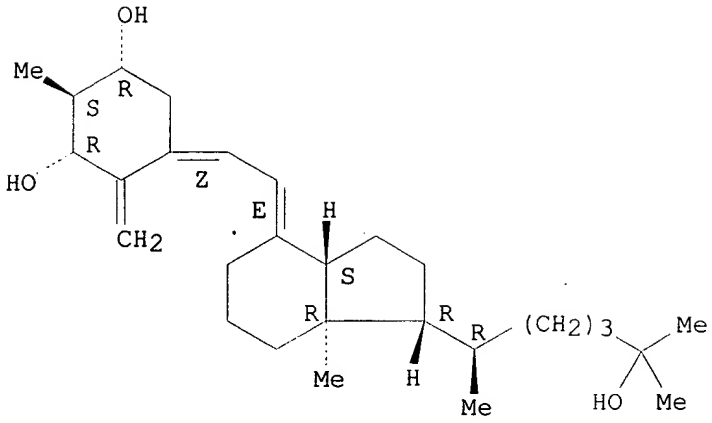

RN 203126-92-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



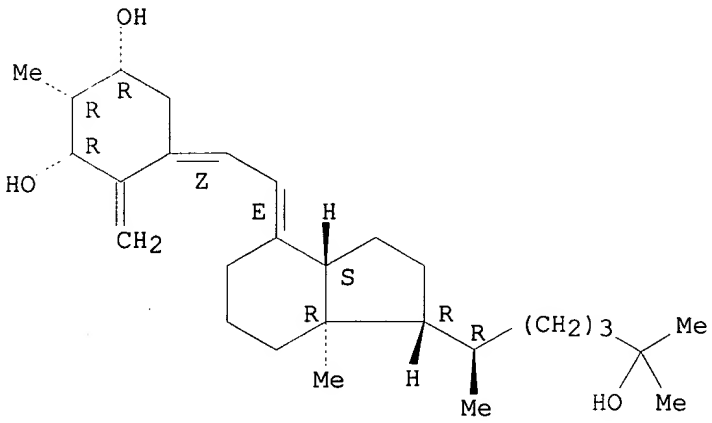

RN 203126-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



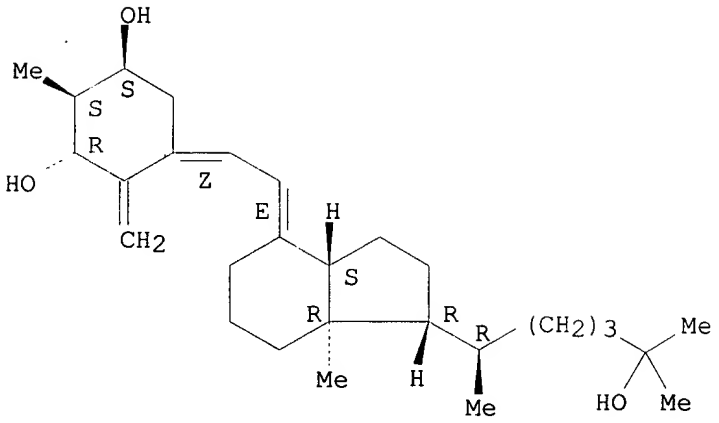

RN 203126-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



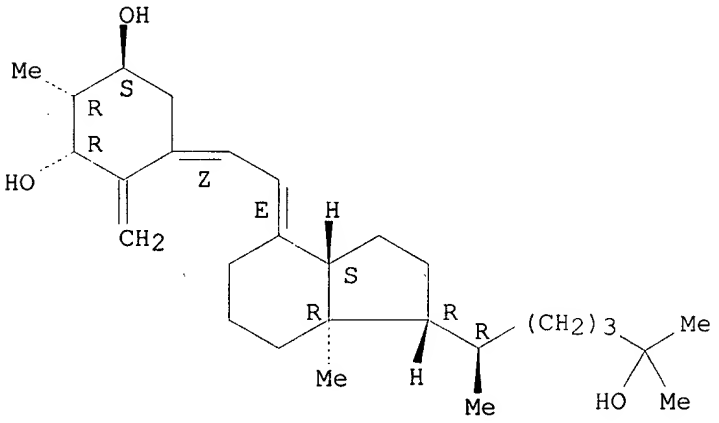

RN 203126-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

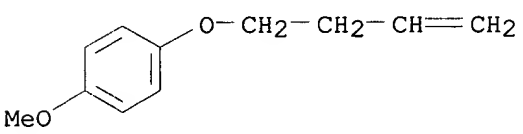


RN 203126-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



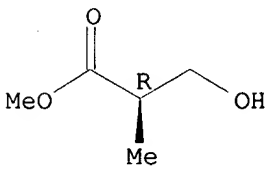
IT **2653-90-9 72657-23-9,** Methyl (R)-3-hydroxy-2-methylpropionate **80657-57-4,** Methyl (S)-3-hydroxy-2-methylpropionate **143705-63-9**
RL: RCT (Reactant)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)
RN 2653-90-9 HCAPLUS
CN Benzene, 1-(3-butenyloxy)-4-methoxy- (7CI, 9CI) (CA INDEX NAME)



RN 72657-23-9 HCAPLUS

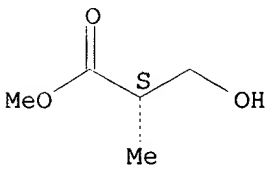
CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



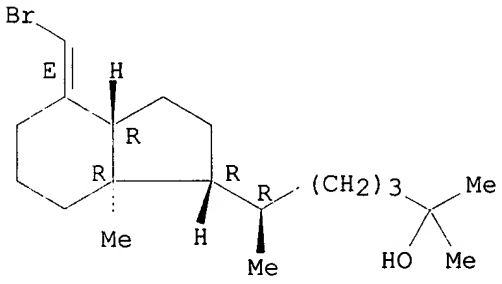

RN 80657-57-4 HCAPLUS
CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).




RN 143705-63-9 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)-(9CI) (CA INDEX NAME)

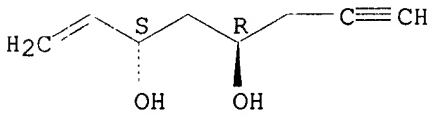
Absolute stereochemistry.
Double bond geometry as shown.




IT **152032-72-9P 161055-41-0P 169310-79-6P**
**169315-01-9P 203126-72-1P 203126-74-3P**
**203126-76-5P 203126-78-7P 203126-79-8P**
**203126-80-1P 203126-81-2P 203126-83-4P**
**203126-84-5P 203126-85-6P 203126-86-7P**
**203126-87-8P 203126-88-9P 203126-89-0P**
**203126-90-3P 203126-97-0P 203126-98-1P**
**203126-99-2P 203127-00-8P 203127-01-9P**
**203127-02-0P 203127-03-1P 203127-04-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)

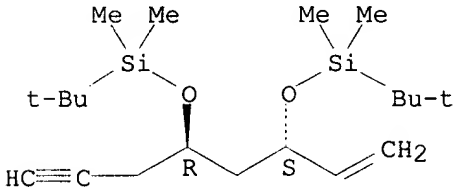
RN 152032-72-9 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



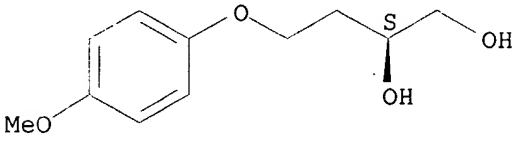
RN 161055-41-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, (5S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



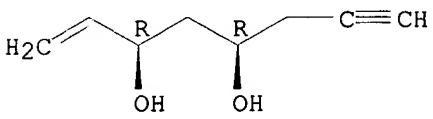
RN 169310-79-6 HCAPLUS
CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



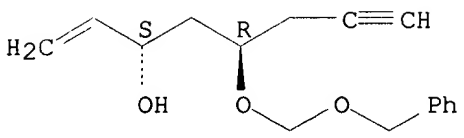
RN 169315-01-9 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



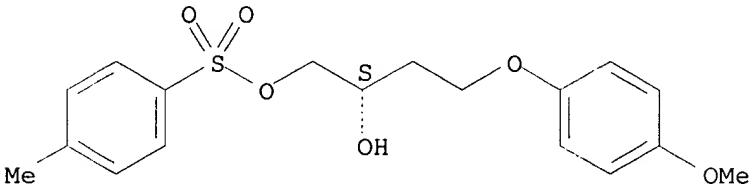
RN 203126-72-1 HCAPLUS
CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



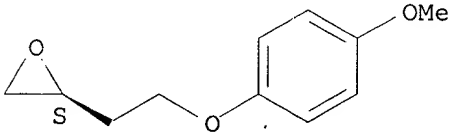
RN 203126-74-3 HCAPLUS
CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, 1-(4-methylbenzenesulfonate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



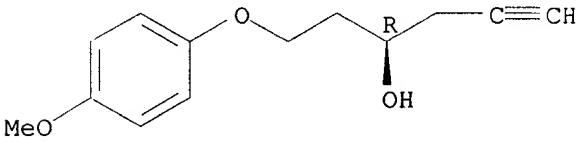
RN 203126-76-5 HCAPLUS
CN Oxirane, [2-(4-methoxyphenoxy)ethyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



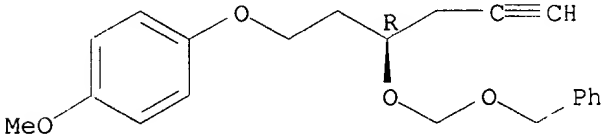
RN 203126-78-7 HCAPLUS
CN 5-Hexyn-3-ol, 1-(4-methoxyphenoxy)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



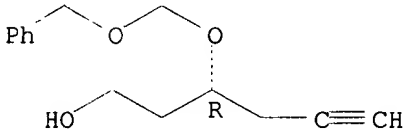
RN 203126-79-8 HCAPLUS
CN Benzene, 1-methoxy-4-[[3-[(phenylmethoxy)methoxy]-5-hexynyl]oxy]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



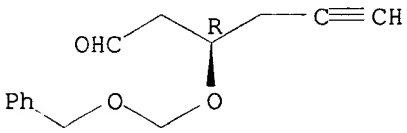
RN 203126-80-1 HCAPLUS
CN 5-Hexyn-1-ol, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



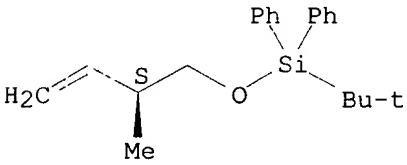
RN 203126-81-2 HCAPLUS
CN 5-Hexynal, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



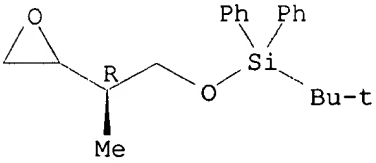
RN 203126-83-4 HCAPLUS
CN Silane, (1,1-dimethylethyl)[(2-methyl-3-butenyl)oxy]diphenyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



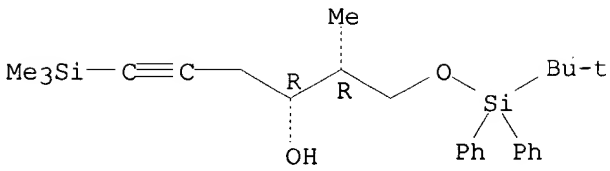
RN 203126-84-5 HCAPLUS
CN Silane, (1,1-dimethylethyl)(2-oxiranylpropoxy)diphenyl-, [2(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



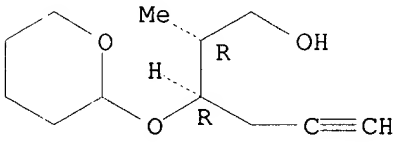
RN 203126-85-6 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



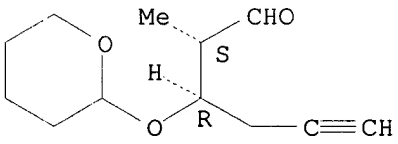
RN 203126-86-7 HCAPLUS
CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, [2(2R,3R)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



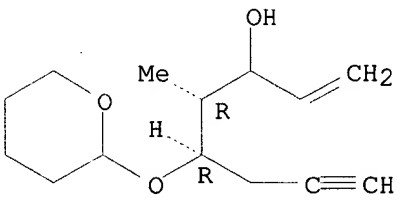
RN 203126-87-8 HCAPLUS
CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, [2(2S,3R)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



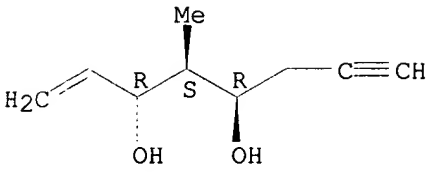
RN 203126-88-9 HCAPLUS
CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, [2(4R,5R)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



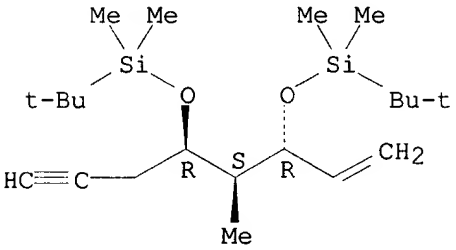
RN 203126-89-0 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, [3R-(3R*,4S*,5R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



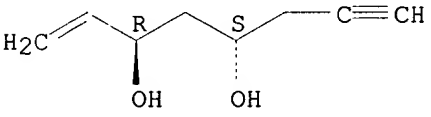
RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



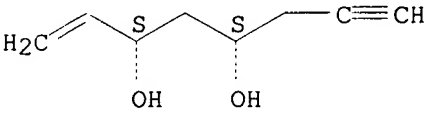
RN 203126-97-0 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



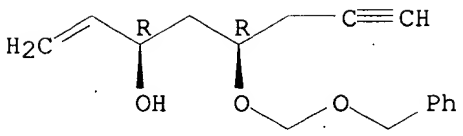
RN 203126-98-1 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



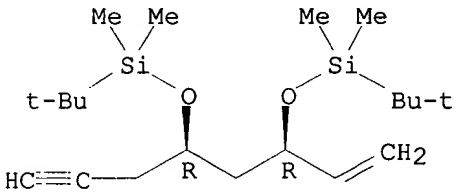
RN 203126-99-2 HCAPLUS
CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



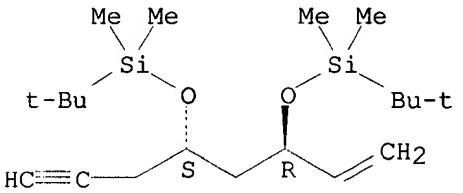
RN 203127-00-8 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



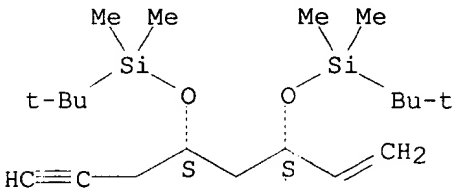
RN 203127-01-9 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



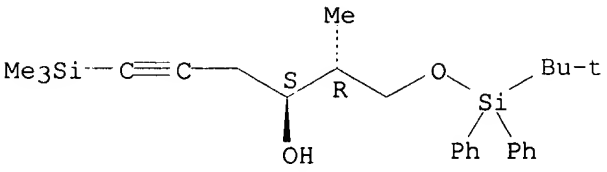
RN 203127-02-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



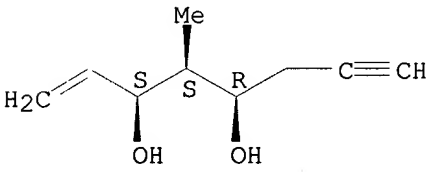
RN 203127-03-1 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



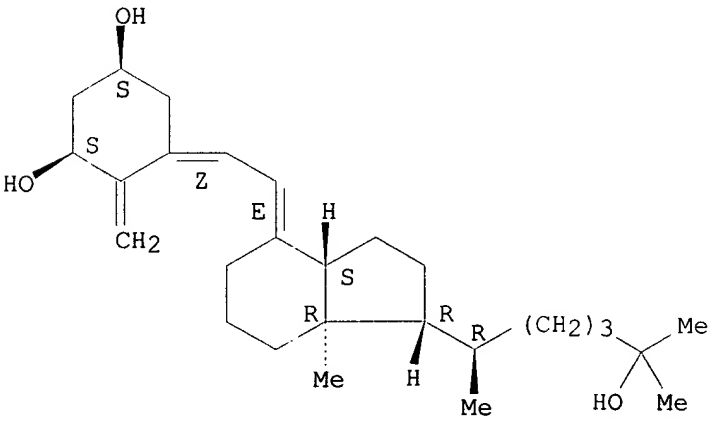
RN 203127-04-2 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, [3S-(3R*,4R*,5S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **61476-45-7P 66791-71-7P 96614-28-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)
RN 61476-45-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

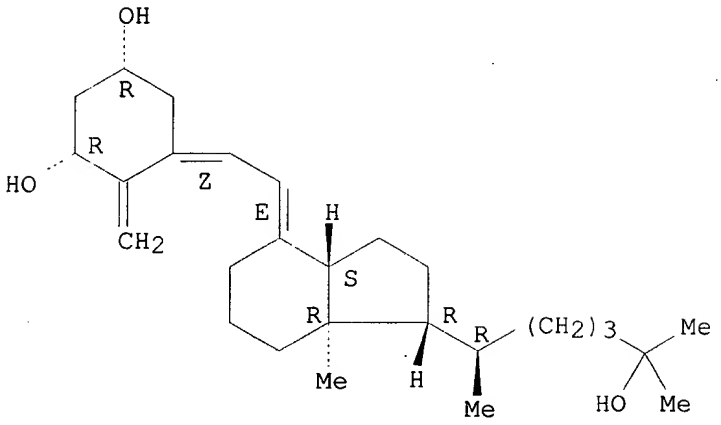
Absolute stereochemistry.
Double bond geometry as shown.



RN 66791-71-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.beta.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

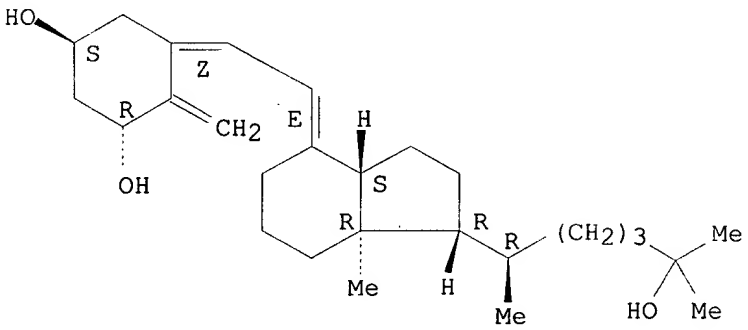
Absolute stereochemistry.

Double bond geometry as shown.




RN 96614-28-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.beta.,3.alpha.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



Beilstein Query



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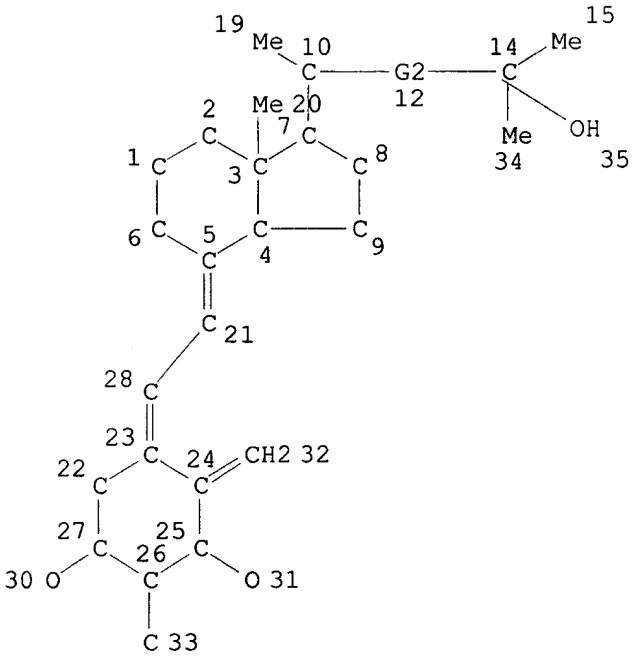
L20 STR




REP G2=(2-4) CH2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE
L21 42 SEA FILE=BEILSTEIN SSS FUL L20
L22 42 SEA FILE=BEILSTEIN ABB=ON PLU=ON L21 AND PRE/FA

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L22 ANSWER 1 OF 42 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 8046533 Beilstein
Molecular Formula (MF): C40 H74 O3 Si2
Autonom Name (AUN):
6-(4-(2-<3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-

methyl-2-methylene-cyclohexylidene>-ethylidene)-7a-
methyl-octahydro-inden-1-yl)-2-methyl-heptan-2-ol
Beilstein Reference (SO): 6-06
General Comments (NTE): Stereo compound
Rltd. Stereoisomers (RSI): 7912362; 7912363; 7912364; 7912365; 7912366;
7912367; 7912368; 7912369; 8046526; 8046527;
8046528; 8046529; 8046530; 8046531; 8046532
Formula Weight (FW): 659.19
Lawson Number (LN): 6523; 3798; 3777

Ring System Data:

Number of Rings (CNR): 3
Ring Systems (CNRS): 2
Diff. Ring Systems (CNDRS): 2
Ring Heteros (CNRH): 0
Acyclic Heteros (CNAH): 5

| Beilstein Ring Index (BRIX) | Ring System Formula (RF) | BRIX Count |
|---|---|---|
| 9.2.5-0.0-0.0 | C9 | 1 |
| 6.1.0-0.0-0.0 | C6 | 1 |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
Atom/Bond Notes:
1. CIP Descriptor: R
2. CIP Descriptor: S
3. CIP Descriptor: E
4. CIP Descriptor: Z

Preparation:
PRE
Start: BRN=7994164
6-(4-bromomethylene-7a-methyl-octahydro-inden-1-yl)-2-
methyl-heptan-2-ol, BRN=7907279 3,5-bis-(tert-butyl-dimethyl-
silanyloxy)-4-methyl-oct-1-en-7-yne
Reag: Pd2(dba)3, Ph3P, Et3N
Solv: CHCl3, toluene
Heating
Reference(s):
1. Fujishima, Toshie; Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Ishizuka, Seiichi; et al., Bioorg.Med.Chem.Lett., 8 <1998> 16, 2145-2148, LA: EN, CODEN: BMCLE8

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L24 ANSWER 1 OF 26 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 7912369 Beilstein
Molecular Formula (MF): C40 H74 O3 Si2
Autonom Name (AUN):
6-(4-(2-<3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-

methyl-2-methylene-cyclohexylidene>-ethylidene)-7a-
methyl-octahydro-inden-1-yl)-2-methyl-heptan-2-ol
Beilstein Reference (SO): 6-06
General Comments (NTE): Stereo compound
Rltd. Stereoisomers (RSI): 7912362; 7912363; 7912364; 7912365; 7912366;
7912367; 7912368; 8046526; 8046527; 8046528;
8046529; 8046530; 8046531; 8046532; 8046533
Formula Weight (FW): 659.19
Lawson Number (LN): 6523; 3798; 3777

Ring System Data:

Number of Rings (CNR): 3
Ring Systems (CNRS): 2
Diff. Ring Systems (CNDRS): 2
Ring Heteros (CNRH): 0
Acyclic Heteros (CNAH): 5

| Beilstein Ring Index (BRIX) | Ring System Formula (RF) | BRIX Count |
|---|---|---|
| 9.2.5-0.0-0.0 | C9 | 1 |
| 6.1.0-0.0-0.0 | C6 | 1 |

Preparation:
PRE
Start: BRN=7907279
3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-methyl-oct-
1-en-7-yne, BRN=5868945 6-(4-bromomethylene-7a-methyl-octahydro-
inden-1-yl)-2-methyl-heptan-2-ol
Reag: Pd2(dba)3PPh3, Et3N
Solv: toluene
Temp: 120.0 Cel
Reference(s):
1. Konno, Katsuhiro; Maki, Shojiro; Fujishima, Toshie; Liu, Zhaopeng; Miura, Daishiro; et al., Bioorg.Med.Chem.Lett., 8 <1998> 2, 151-156, LA: EN, CODEN: BMCLE8

=> d

L27 ANSWER 1 OF 10 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 7837289 Beilstein
Molecular Formula (MF): C33 H56 O4
Autonom Name (AUN): 5-(2-<1-(5-hydroxy-1,5-dimethyl-hexyl)-7a-methyl-octahydro-inden-4-ylidene>-ethylidene)-2-(6-hydroxy-hexyl)-4-methylene-cyclohexane-1,3-diol
Beilstein Reference (SO): 6-06
General Comments (NTE): Stereo compound
Formula Weight (FW): 516.80
Lawson Number (LN): 6704

Ring System Data:

Number of Rings (CNR): 3
Ring Systems (CNRS): 2
Diff. Ring Systems (CNDRS): 2
Ring Heteros (CNRH): 0
Acyclic Heteros (CNAH): 4

| Beilstein Ring Index (BRIX) | Ring System Formula (RF) | BRIX Count |
|---|---|---|
| 9.2.5-0.0-0.0 | C9 | 1 |
| 6.1.0-0.0-0.0 | C6 | 1 |

Preparation:
PRE
Start: BRN=7836562 (2R)-2-(6-hydroxyhexyl)-1.alpha.,3.beta.,25-trihydroxycholesta-5,7-diene
Detail: 1.) EtOH, 0 deg C, 2 min, irrad. 2.) EtOH, 2 h, reflux
Reference(s):
1. Ono, Yoshiyuki; Watanabe, Hiroyoshi; Shiraishi, Ayako; Takeda, Satoshi; Higuchi, Yoshinobu; et al., Chem.Pharm.Bull., 45 <1997> 10, 1626-1630, LA: EN, CODEN: CPBTAL
Note(s):
2. Yield given. Multistep reaction

=> d

L30 ANSWER 1 OF 5 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 7343182 Beilstein
Molecular Formula (MF): C31 H51 F O3
Autonom Name (AUN):
2-(4-fluoro-butyl)-5-(2-<1-(5-hydroxy-1,5-dimethyl-hexyl)-7a-methyl-octahydro-inden-4-ylidene>-ethylidene)-4-methylene-cyclohexane-1,3-diol
Beilstein Reference (SO): 6-06
General Comments (NTE): Stereo compound
Rltd. Stereoisomers (RSI): 7343181
Formula Weight (FW): 490.74
Lawson Number (LN): 6526

Ring System Data:

Number of Rings (CNR): 3
Ring Systems (CNRS): 2
Diff. Ring Systems (CNDRS): 2
Ring Heteros (CNRH): 0
Acyclic Heteros (CNAH): 4

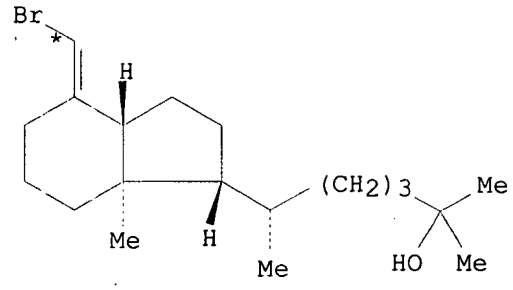
| Beilstein Ring Index (BRIX) | Ring System Formula (RF) | BRIX Count |
|---|---|---|
| 9.2.5-0.0-0.0 | C9 | 1 |
| 6.1.0-0.0-0.0 | C6 | 1 |

Preparation:
PRE
Start: BRN=7326668 4-(2-<3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-(4-fluoro-butyl)-2-methylene-cyclohexylidene>-ethylidene)-1-<5-(tert-butyl-dimethyl-silanyloxy)-1,5-dimethyl-hexyl>-7a-methyl-octahydro-indene
Reag: n-Bu4NF, 4 Angstroem molecular sieves
Time: 3.5 hour(s)
Solv: tetrahydrofuran
Temp: 60.0 Cel
ByProd: BRN=7343181 2-(4-fluoro-butyl)-5-(2-<1-(5-hydroxy-1,5-dimethyl-hexyl)-7a-methyl-octahydro-inden-4-ylidene>-ethylidene)-4-methylene-cyclohexane-1,3-diol
Reference(s):
1. Posner, Gary H.; Cho, Cheon-Gyu; Anjeh, Tizah E. N.; Johnson, Neil; Horst, Ronald L.; et al., J.Org.Chem., 60 <1995> 14, 4617-4628, LA: EN,
CODEN: JOCEAH
Note(s):
2. Yield given. Yields of byproduct given

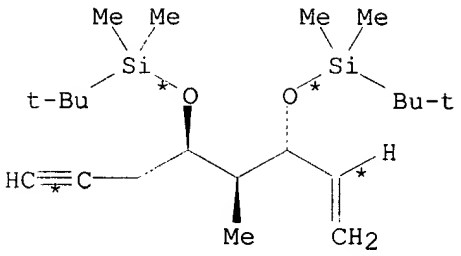
=> d fhit bib abs

L38 ANSWER 1 OF 1 CASREACT COPYRIGHT 1999 ACS

RX(1) OF 1 **A** + B ===> **C**

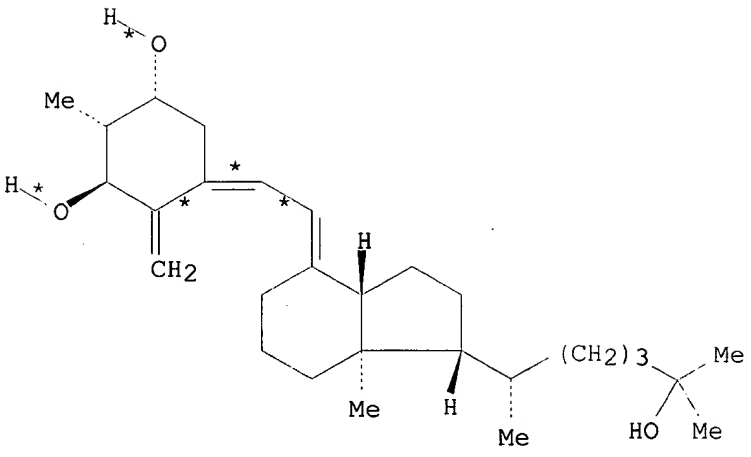


A



B

(1)



C

RX(1) RCT A **214351-89-0**, B 203126-90-3
RGT D 121-44-8 Et3N, E 603-35-0 PPh3
PRO C **214351-93-6**
CAT 52522-40-4 Pd complex
SOL 108-88-3 PhMe

AN 129:343629 CASREACT

TI Preparation of vitamin D3 derivatives and their pharmaceutical uses

IN Takayama, Hiroaki; Konno, Katsuhiro; Fujishima, Toshie
PA Teijin Ltd., Japan
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9850353 | A1 | 19981112 | WO 98-JP1979 | 19980430 |
| | W: JP, US | | | | |
| | RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |

PRAI JP 97-114695 19970502
OS MARPAT 129:343629
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-Me vitamin D3 derivs. I [R1, R2 = H, tri(C1-7alkyl)silyl; the asym. carbon atoms at the 1-, 2- and 3-positions each independently has an .alpha.- or .beta.-configuration], useful as remedies for osteoporosis, rachitis, accessory thyroidal hyperenergia, etc., are prepd. via reaction of II (X = bromo, iodo) with III (R3, R4 = H, trihydrocarbylsilyl) in the presence of a palladium catalyst optionally followed by deprotection (removal of silyl groups). Thus, II (X = Br) was reacted with III (R3 = R4 = TBS) in toluene contg. Et3N, Pd2(dba)3.CHCl3, and Ph3P at 120.degree. to give IV (R = TBS), which was treated with camphor-10-sulfonic acid in methanol to give 63% IV (R = H). In a study using 1.alpha.,25-dihydroxyvitamin D3 receptors in the bovine thymus gland, this showed an affinity of 160 compared with 100 for 1.alpha.,25-dihydroxyvitamin D3.

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=> D HIS


     (FILE 'HOME' ENTERED AT 14:02:27 ON 22 JUN 1999)

     FILE 'HCAPLUS' ENTERED AT 14:02:33 ON 22 JUN 1999
L1           719 S TAKAYAMA H?/AU
L2           896 S KONNO K?/AU
L3           172 S FUJISHIMA T?/AU
L4             4 S L1 AND L2 AND L3
                 SELECT RN L4 1-4

     FILE 'HCAPLUS' ENTERED AT 14:03:07 ON 22 JUN 1999

     FILE 'REGISTRY' ENTERED AT 14:03:23 ON 22 JUN 1999
L5            96 S E1-96

     FILE 'HCAPLUS' ENTERED AT 14:03:41 ON 22 JUN 1999
L6             3 S L4 AND L5
L7             1 S L4 NOT L6
```

=> D ALL

L7 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:710271 HCAPLUS
TI Corrigendum to "A novel and practical route to A-ring enyne synthon for 1.alpha.,25-dihydroxyvitamin D3 analogs: synthesis of A-ring diastereomers of 1.alpha.,25-dihydroxy-vitamin D3 and 2-methyl-1,25-dihydroxyvitamin D3"
AU **Konno, Katsuhiro**; Maki, Shojiro; **Fujishima, Toshie**; Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; **Takayama, Hiroaki**
CS Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko, Kanagawa, 199-01, Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(19), 2817
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal; Errata
LA English
AB Unavailable

=> D L6 BIB ABS HITSTR

L6 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:745027 HCAPLUS
DN 129:343629
TI Preparation of vitamin D3 derivatives and their pharmaceutical uses
IN **Takayama, Hiroaki; Konno, Katsuhiro; Fujishima, Toshie**
PA Teijin Ltd., Japan
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 2

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 9850353 | A1 | 19981112 | WO 98-JP1979 | 19980430 |

W: JP, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

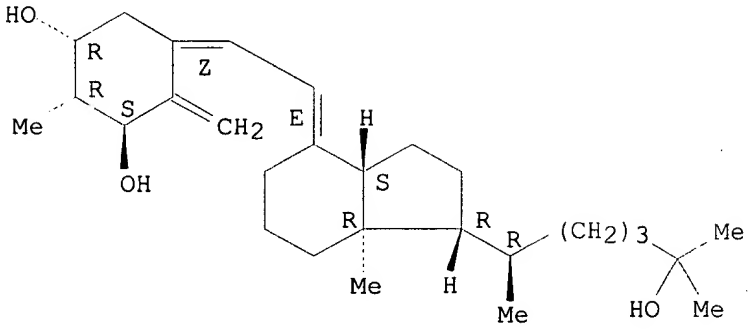
PRAI JP 97-114695 19970502
OS CASREACT 129:343629; MARPAT 129:343629
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-Me vitamin D3 derivs. I [R1, R2 = H, tri(C1-7alkyl)silyl; the asym. carbon atoms at the 1-, 2- and 3-positions each independently has an .alpha.- or .beta.-configuration], useful as remedies for osteoporosis, rachitis, accessory thyroidal hyperenergia, etc., are prepd. via reaction of II (X = bromo, iodo) with III (R3, R4 = H, trihydrocarbylsilyl) in the presence of a palladium catalyst optionally followed by deprotection (removal of silyl groups). Thus, II (X = Br) was reacted with III (R3 = R4 = TBS) in toluene contg. Et3N, Pd2(dba)3.CHCl3, and Ph3P at 120.degree. to give IV (R = TBS), which was treated with camphor-10-sulfonic acid in methanol to give 63% IV (R = H). In a study using 1.alpha.,25-dihydroxyvitamin D3 receptors in the bovine thymus gland, this showed an affinity of 160 compared with 100 for 1.alpha.,25-dihydroxyvitamin D3.
IT **158388-11-5P 214351-93-6P 214351-94-7P 214351-95-8P 214351-96-9P 214351-97-0P 214351-98-1P 214351-99-2P 215394-65-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 158388-11-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

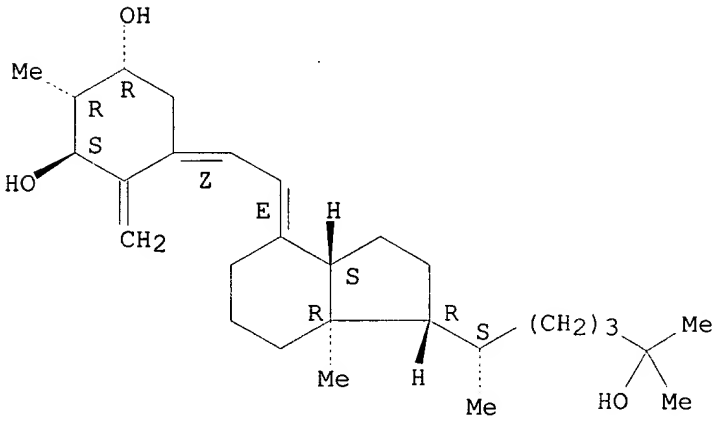
Absolute stereochemistry.

Double bond geometry as shown.



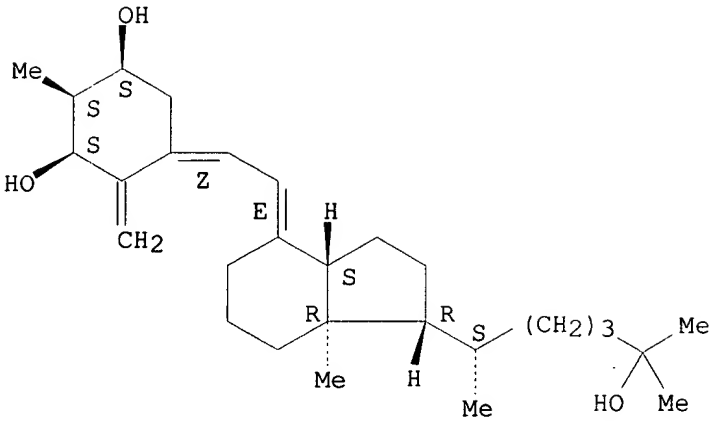

RN 214351-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



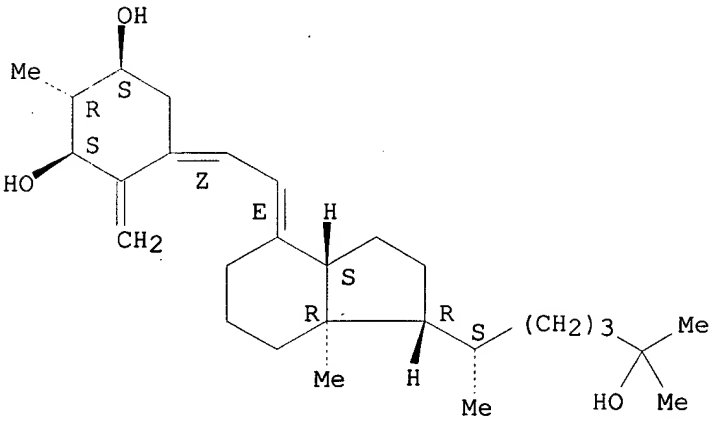

RN 214351-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



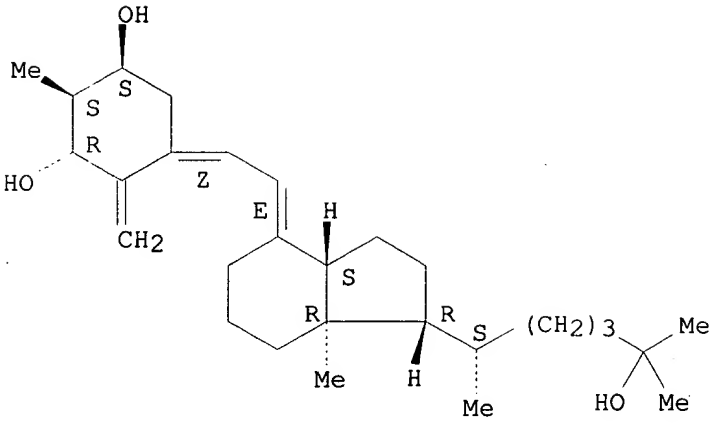

RN 214351-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



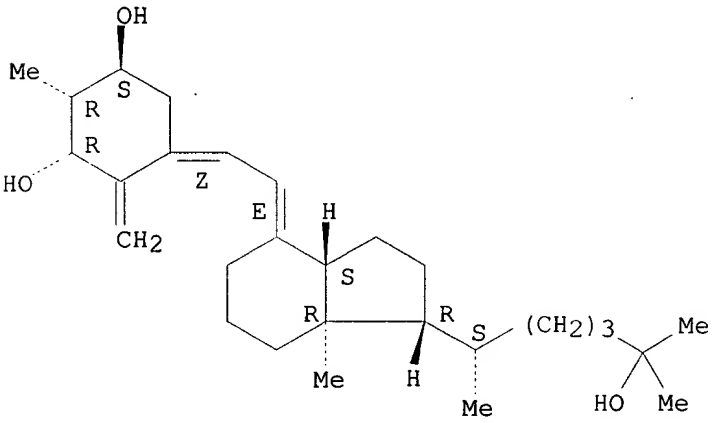

RN 214351-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



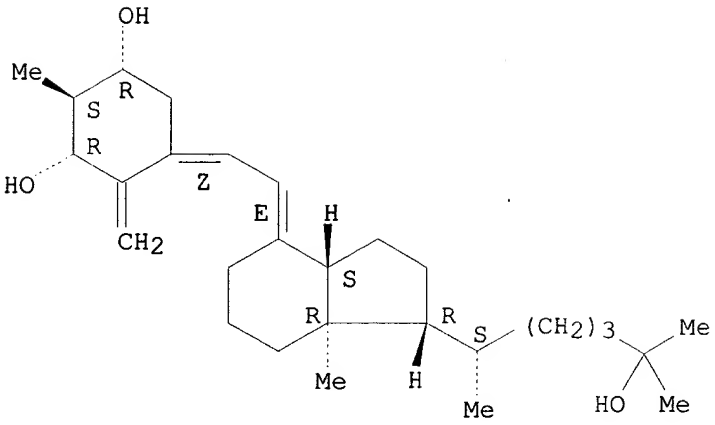
RN 214351-97-0 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



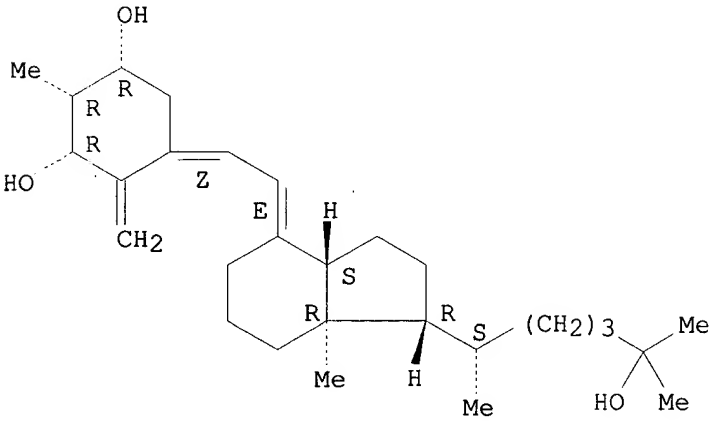
RN 214351-98-1 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



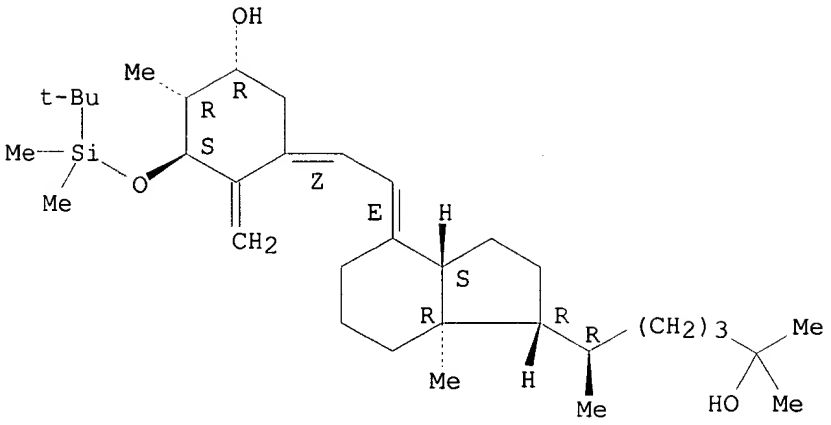
RN 214351-99-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 215394-65-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-3,25-triol, 1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

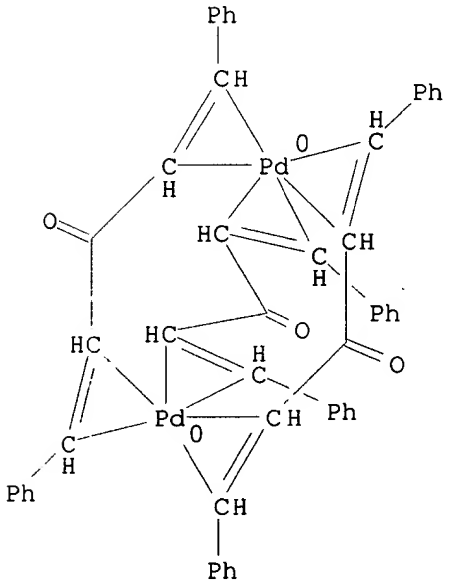
Absolute stereochemistry.
Double bond geometry as shown.



IT **52522-40-4**
RL: CAT (Catalyst use); USES (Uses)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 52522-40-4 HCAPLUS
CN Palladium, tris[.mu.-[(1,2-.eta.:4,5-.eta.)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]di-, compd. with trichloromethane (1:1) (9CI) (CA INDEX NAME)

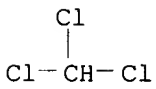
CM 1

CRN 51364-51-3
CMF C51 H42 O3 Pd2
CCI CCS
CDES 2:ALL,E

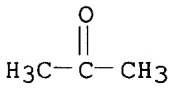


CM 2

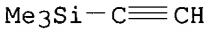
CRN 67-66-3
CMF C H Cl3



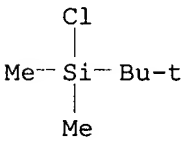
IT **67-64-1**, 2-Propanone, reactions **1066-54-2**, Ethynyltrimethylsilane **18162-48-6**, tert-Butyldimethylsilyl chloride **20445-33-4 39637-99-5 69739-34-0**, tert-Butyldimethylsilyl triflate **143705-63-9 214351-89-0**
RL: RCT (Reactant)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

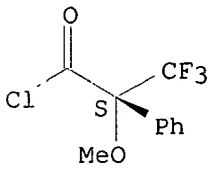


RN 18162-48-6 HCAPLUS
CN Silane, chloro(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 20445-33-4 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (.alpha.S)- (9CI) (CA INDEX NAME)

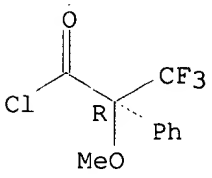
Absolute stereochemistry. Rotation (+).



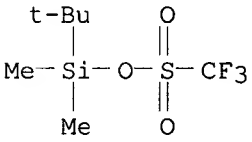
RN 39637-99-5 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,

(.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

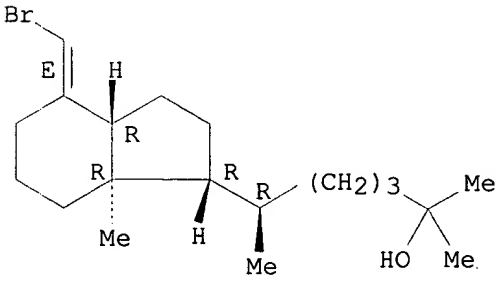


RN 69739-34-0 HCAPLUS
CN Methanesulfonic acid, trifluoro-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)



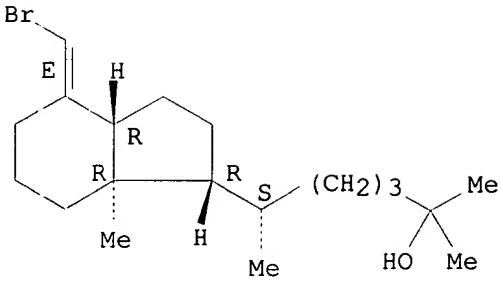
RN 143705-63-9 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-89-0 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

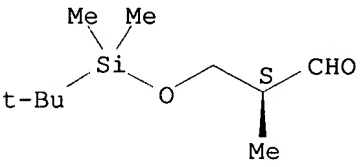
Absolute stereochemistry.
Double bond geometry as shown.




IT **104701-87-3P 112057-64-4P 147915-53-5P**
**147915-54-6P 203126-90-3P 215394-09-5P**
**215394-10-8P 215394-12-0P 215394-15-3P**
**215394-17-5P 215394-20-0P 215394-22-2P**
**215394-23-3P 215394-24-4P 215394-25-5P**
**215394-26-6P 215394-27-7P 215394-28-8P**
**215394-29-9P 215394-30-2P 215394-31-3P**
**215394-32-4P 215394-33-5P 215394-34-6P**
**215394-35-7P 215394-36-8P 215394-37-9P**
**215394-38-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)

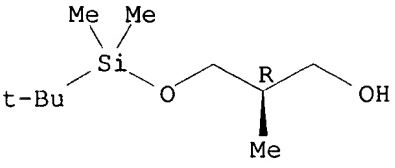
RN 104701-87-3 HCAPLUS
CN Propanal, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.



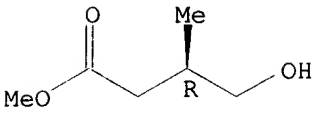

RN 112057-64-4 HCAPLUS
CN 1-Propanol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



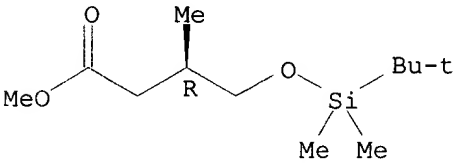

RN 147915-53-5 HCAPLUS
CN Butanoic acid, 4-hydroxy-3-methyl-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



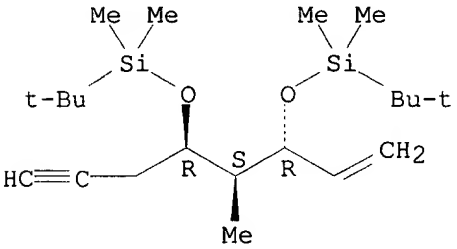
RN 147915-54-6 HCAPLUS
CN Butanoic acid, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methyl-, methyl
ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



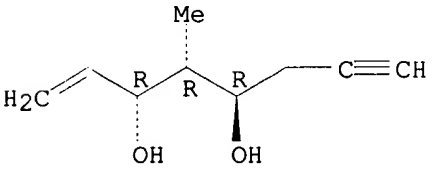
RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



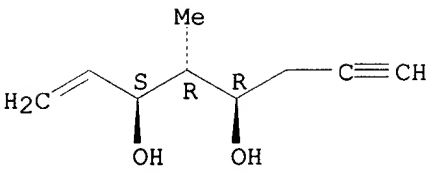
RN 215394-09-5 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



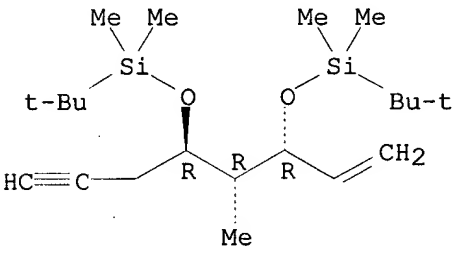
RN 215394-10-8 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3S,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



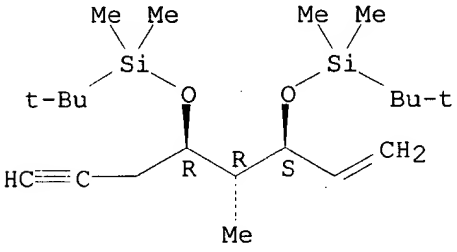
RN 215394-12-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



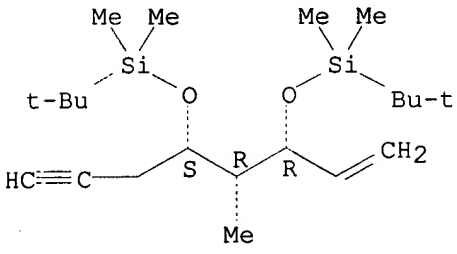
RN 215394-15-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



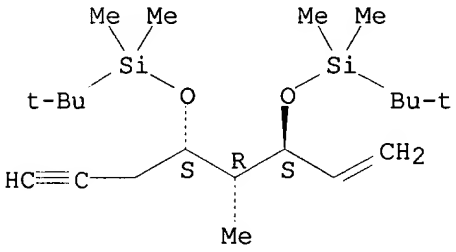
RN 215394-17-5 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



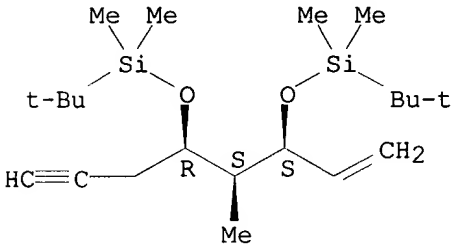
RN 215394-20-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



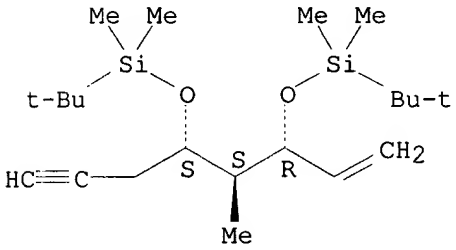

RN 215394-22-2 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



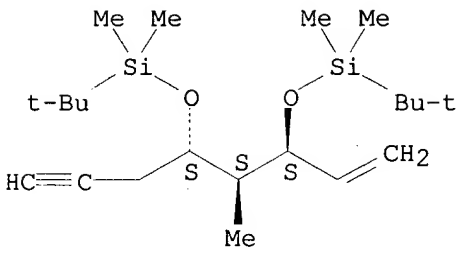

RN 215394-23-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



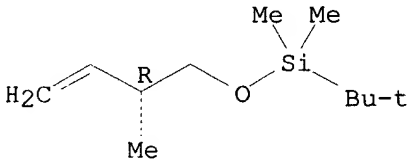

RN 215394-24-4 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



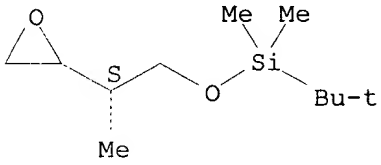
RN 215394-25-5 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(2R)-2-methyl-3-butenyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



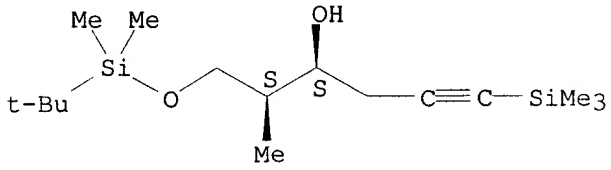
RN 215394-26-6 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[(2S)-2-oxiranylpropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



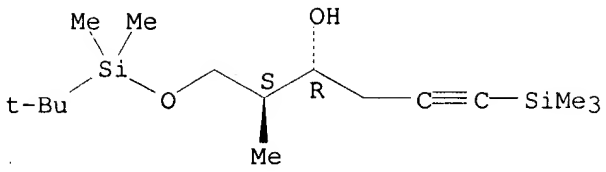
RN 215394-27-7 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



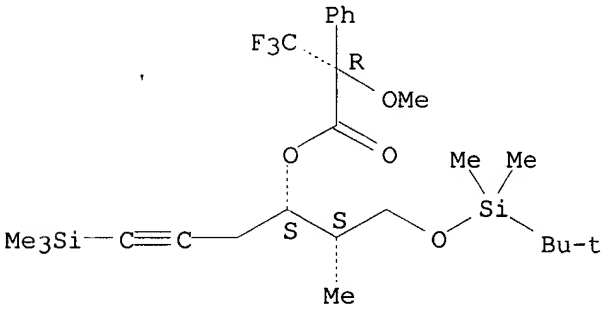
RN 215394-28-8 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



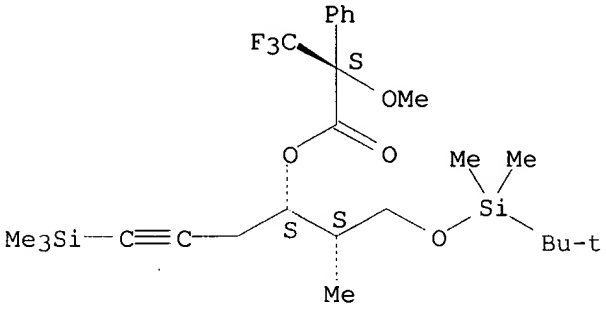
RN 215394-29-9 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



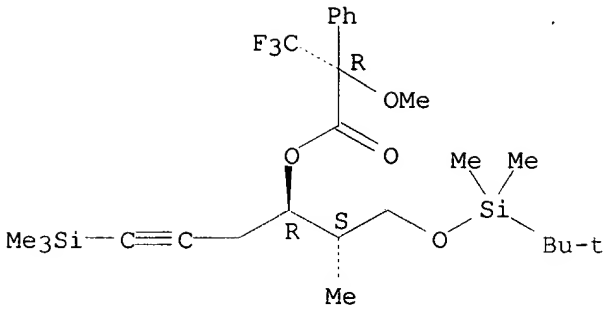
RN 215394-30-2 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



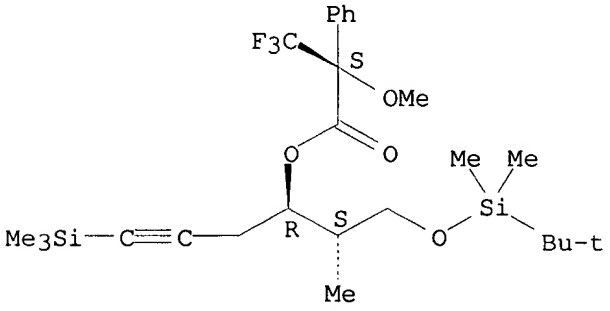
RN 215394-31-3 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



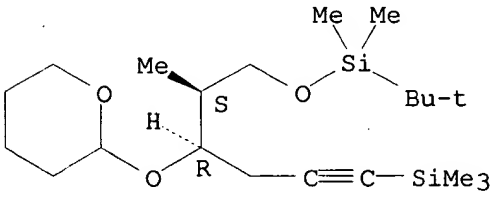
RN 215394-32-4 HCAPLUS
CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



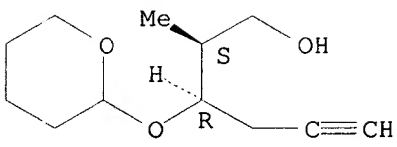
RN 215394-33-5 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[(2S,3R)-2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-3-[3-(trimethylsilyl)-2-propynyl]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



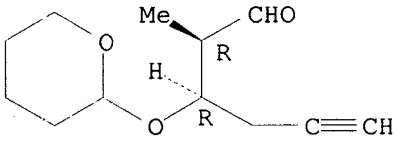
RN 215394-34-6 HCAPLUS
CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



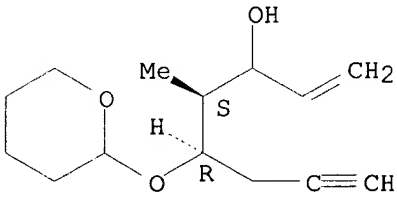

RN 215394-35-7 HCAPLUS
CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



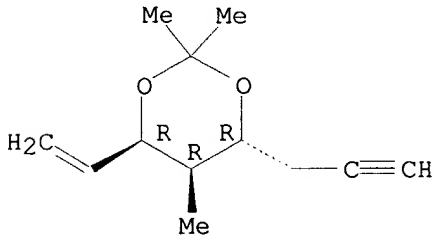

RN 215394-36-8 HCAPLUS
CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



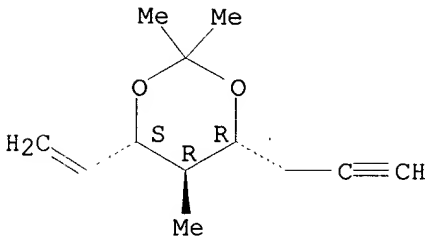

RN 215394-37-9 HCAPLUS
CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4R,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 215394-38-0 HCAPLUS
CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4S,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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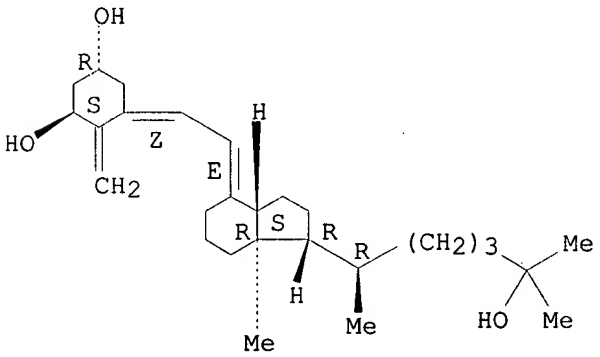
=> D L6 BIB ABS HITSTR 2

L6 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:606883 HCAPLUS
DN 129:290279
TI Synthesis and biological activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3
AU **Fujishima, Toshie;** Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Ishizuka, Seiichi; **Konno, Katsuhiro; Takayama, Hiroaki**
CS Faculty of Pharmaceutical Sciences, Teikyo University, Kanagawa, 199-0195, Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(16), 2145-2148
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB Synthesis and biol. evaluation of all eight possible A-ring diastereomers of 2-methyl-20-epi-1,25-dihydroxyvitamin D3 are described. Among the analogs synthesized, 2.alpha.-methyl-20-epi-1.alpha.,25-dihydroxyvitamin D3 exhibited exceptionally high potency. The double modification of 2-Me substitution and 20-epimerization yielded analogs with unique activity profiles.
IT **32222-06-3P**, 1.alpha.,25-Dihydroxyvitamin D3
RL: PNU (Preparation, unclassified); PREP (Preparation)
(Synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)
RN 32222-06-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

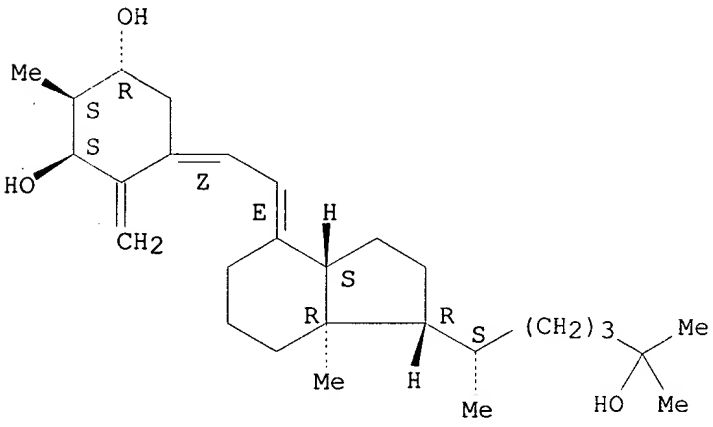



IT **214351-84-5P 214351-93-6P 214351-94-7P 214351-95-8P 214351-96-9P 214351-97-0P 214351-98-1P 214351-99-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. activity of 2-methyl-20-epi analogs of

1.alpha.,25-dihydroxyvitamin D3)

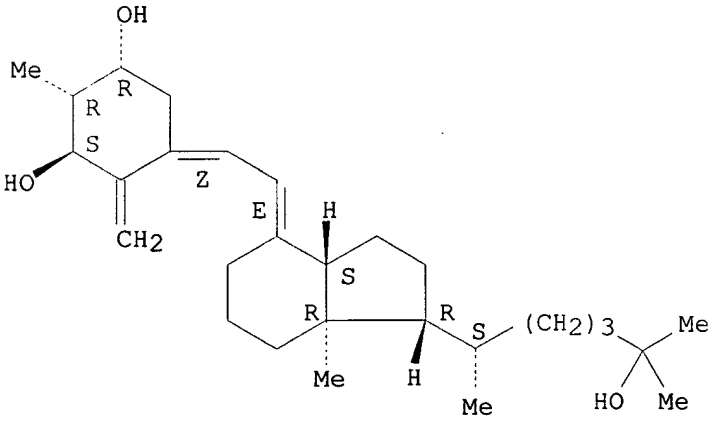
RN 214351-84-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



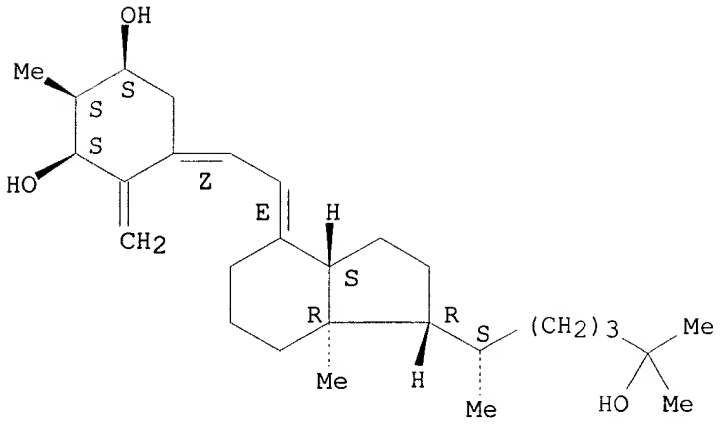
RN 214351-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



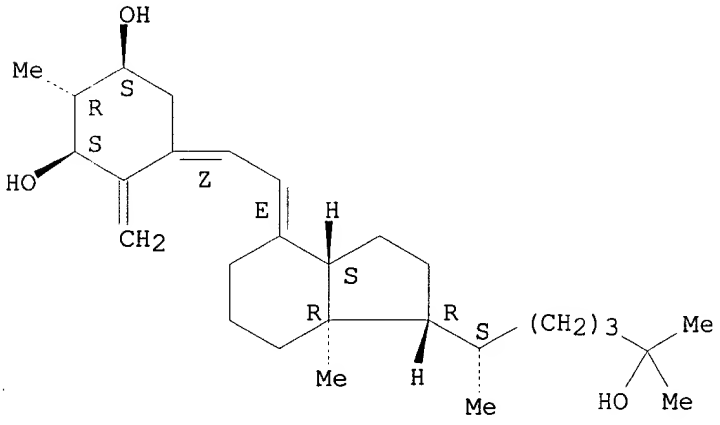
RN 214351-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



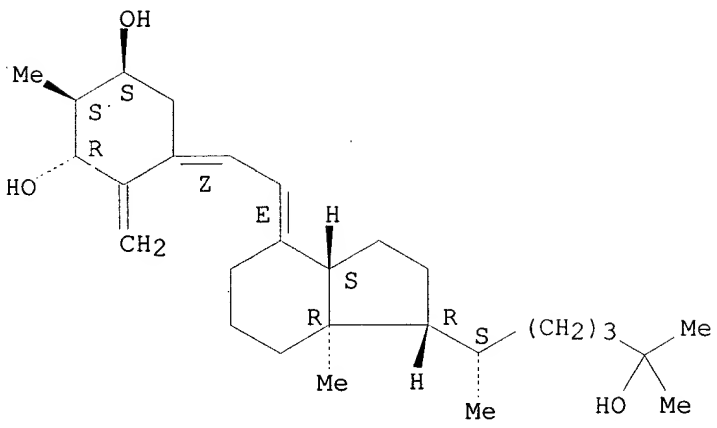

RN 214351-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



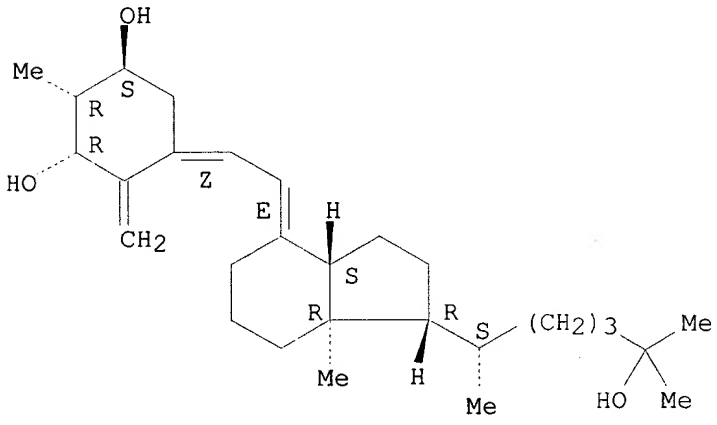

RN 214351-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



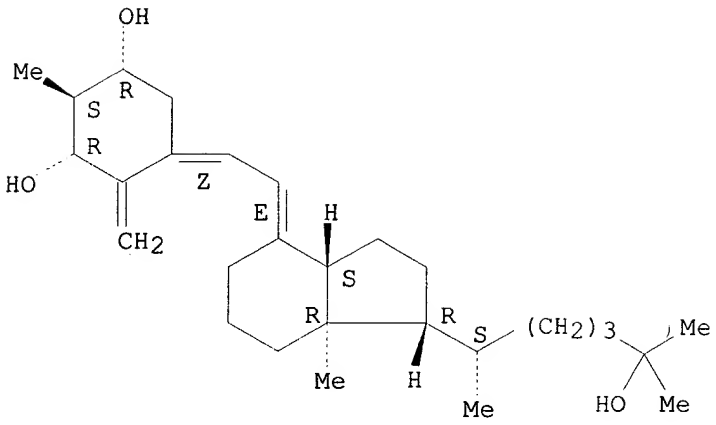

RN 214351-97-0 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



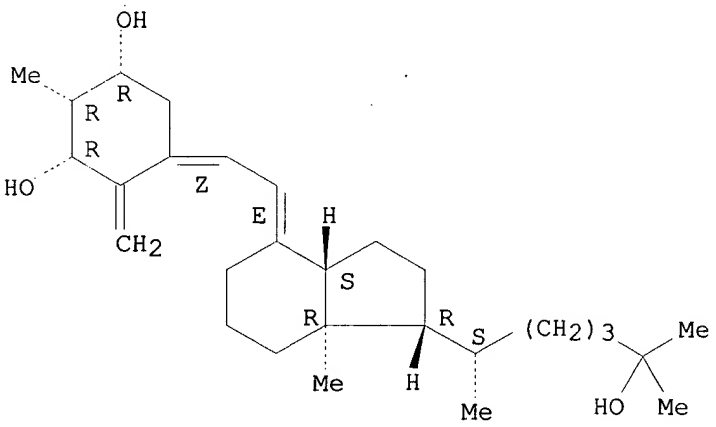

RN 214351-98-1 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



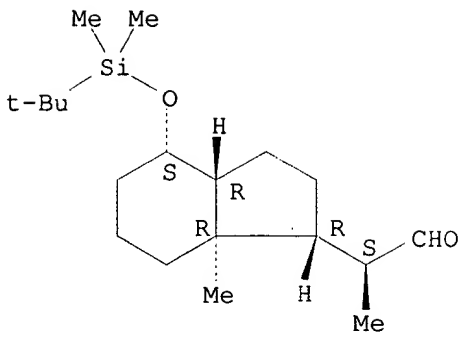
RN 214351-99-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



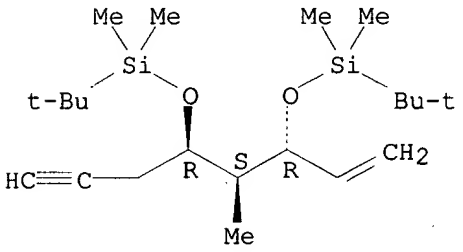
IT **104651-47-0 203126-90-3 214351-87-8**
RL: RCT (Reactant)
(synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)
RN 104651-47-0 HCAPLUS
CN 1H-Indene-1-acetaldehyde, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.alpha.,7a-dimethyl-, (.alpha.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

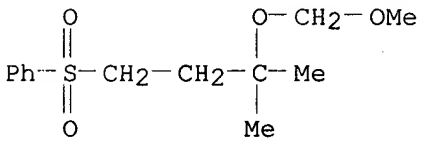


RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

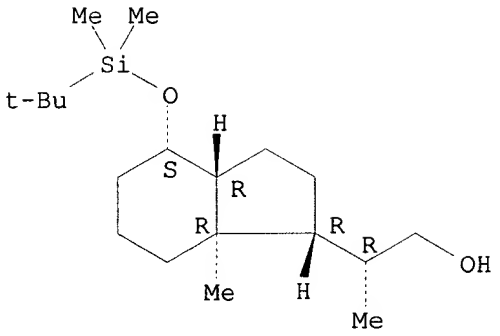


RN 214351-87-8 HCAPLUS
CN Benzene, [[3-(methoxymethoxy)-3-methylbutyl]sulfonyl]- (9CI) (CA INDEX NAME)



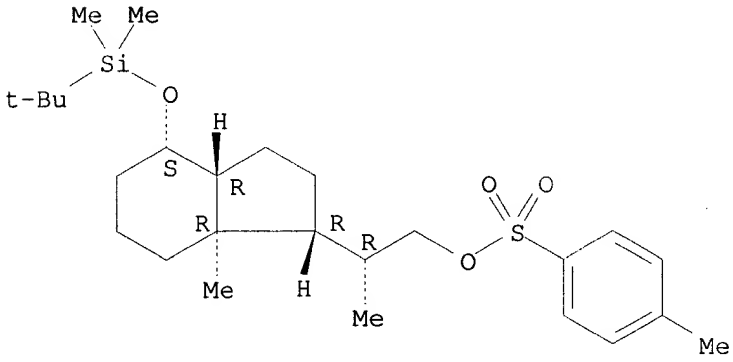
IT **171011-48-6P 183506-75-4P 213250-67-0P**
**214351-86-7P 214351-88-9P 214351-89-0P**
**214351-91-4P 214351-92-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)
RN 171011-48-6 HCAPLUS
CN 1H-Indene-1-ethanol, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, (.beta.R,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



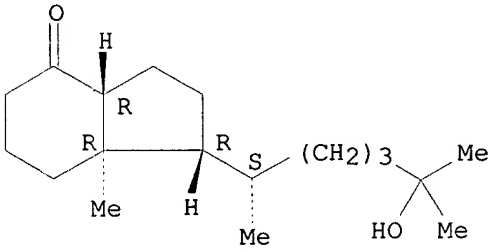
RN 183506-75-4 HCAPLUS
CN 1H-Indene-1-ethanol, 4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, 4-methylbenzenesulfonate, (.beta.R,1R,3aR,4S,7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



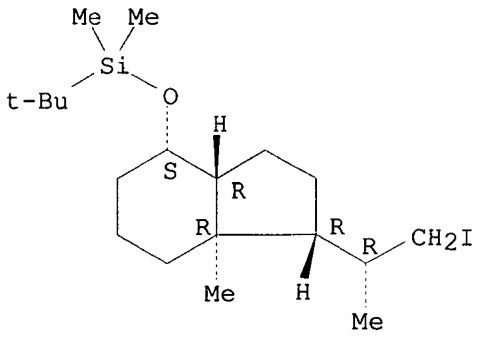
RN 213250-67-0 HCAPLUS
CN 4H-Inden-4-one,
octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-,
(1R,3aR,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



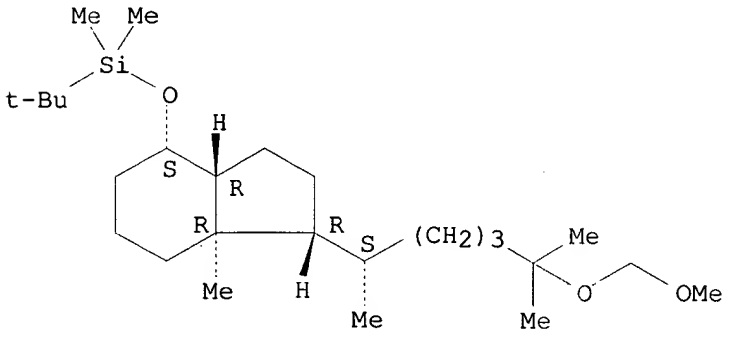
RN 214351-86-7 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-2-iodo-1-methylethyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



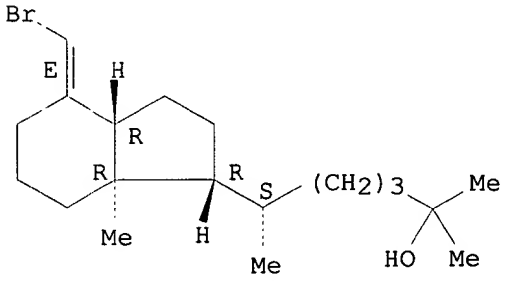
RN 214351-88-9 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1S)-5-(methoxymethoxy)-1,5-dimethylhexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214351-89-0 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)-(9CI) (CA INDEX NAME)

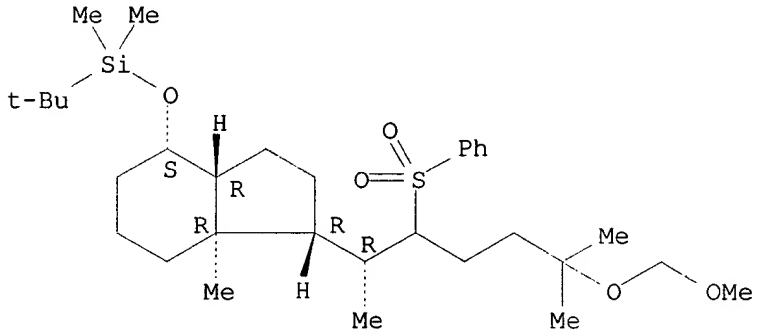
Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-91-4 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-5-

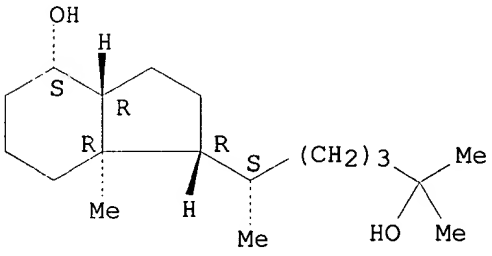
(methoxymethoxy)-1,5-dimethyl-2-(phenylsulfonyl)hexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



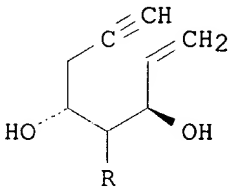

RN 214351-92-5 HCAPLUS
CN 1H-Indene-1-pentanol, octahydro-4-hydroxy-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> D L6 BIB ABS HITSTR 3

L6 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:85846 HCAPLUS
DN 128:180577
TI A novel and practical route to A-ring enyne synthon for 1.alpha.,25-dihydroxyvitamin D3 analogs: synthesis of A-ring diastereomers of 1.alpha.,25-dihydroxyvitamin D3 and 2-methyl-1,25-dihydroxyvitamin D3
AU **Konno, Katsuhiro;** Maki, Shojiro; **Fujishima, Toshie;** Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; **Takayama, Hiroaki**
CS Faculty Pharmaceutical Sciences, Teikyo Univ., Sagamiko, Kanagawa, 199-01, Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(2), 151-156
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 128:180577
GI

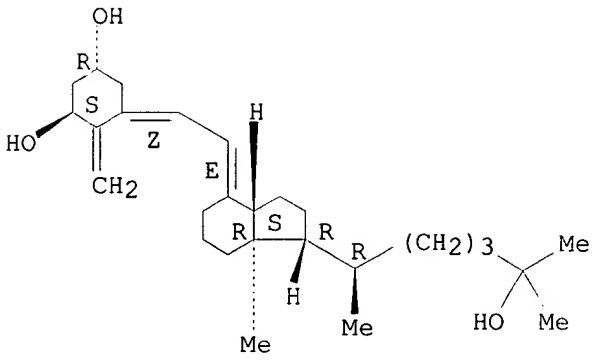



II

AB A novel and practical route to the A-ring enyne synthon II (R = H, Me), which can be versatile for a variety of A-ring analogs of 1.alpha.,25-dihydroxyvitamin D3 (I), was developed. This novel method led to an improved synthesis of the A-ring diastereomers of I, and synthesis of the new analogs, 2-methyl-1,25-dihydroxyvitamin D3 with its all possible diastereomers. The biol. evaluation of the 2-Me analogs showed the .alpha..alpha..beta.-isomer to be more potent than I.

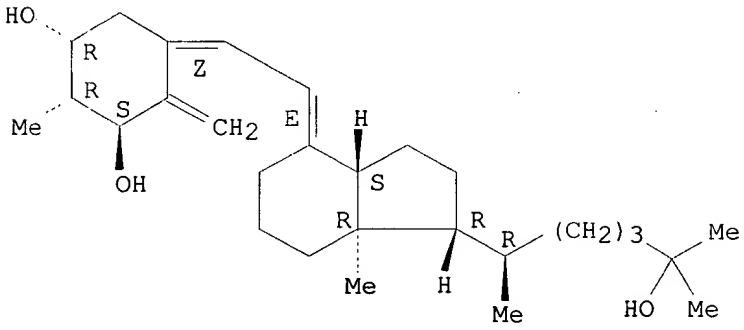
IT **32222-06-3DP**, 1.alpha.,25-Dihydroxyvitamin D3, A-ring analogs **158388-11-5P 203126-73-2P 203126-91-4P 203126-92-5P 203126-93-6P 203126-94-7P 203126-95-8P 203126-96-9P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)
RN 32222-06-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



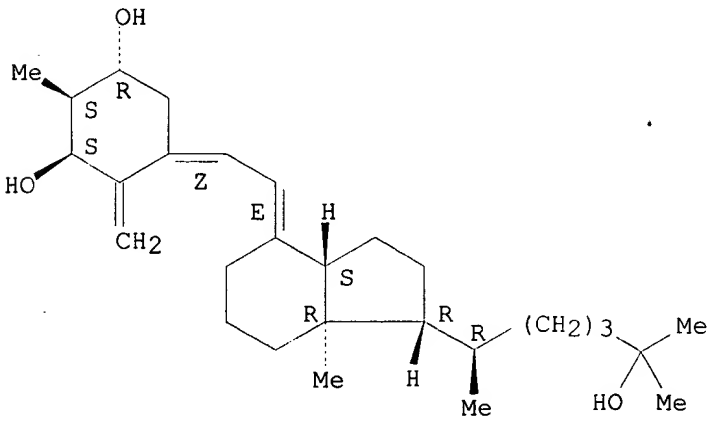
RN 158388-11-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



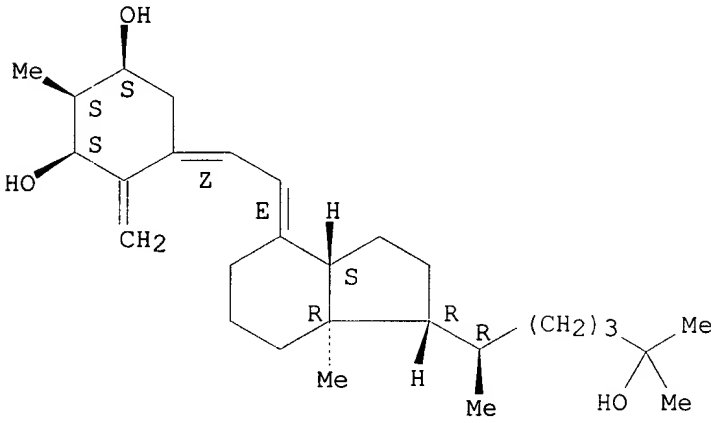
RN 203126-73-2 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



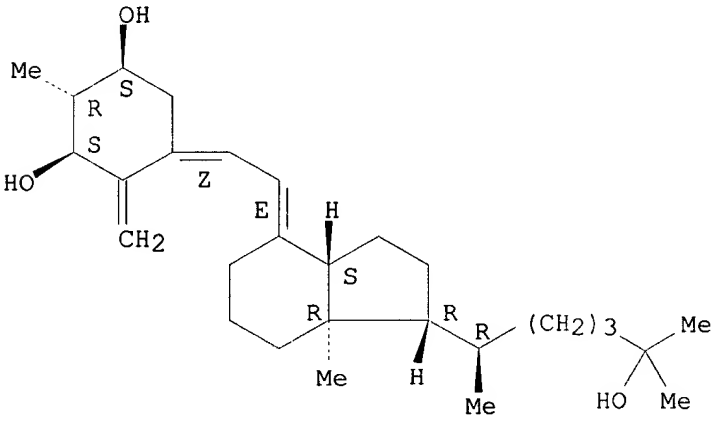
RN 203126-91-4 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



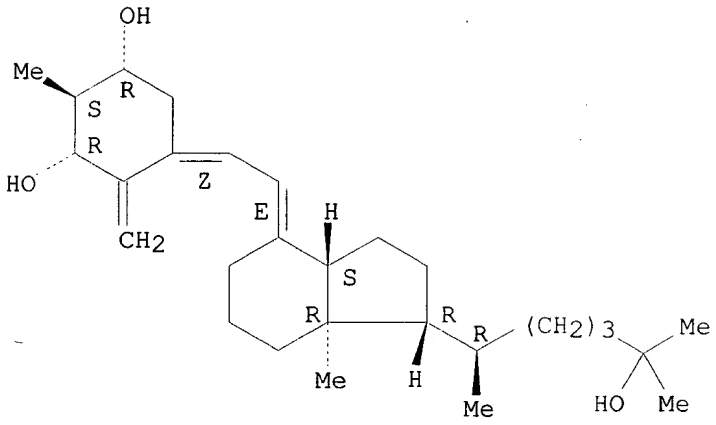

RN 203126-92-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



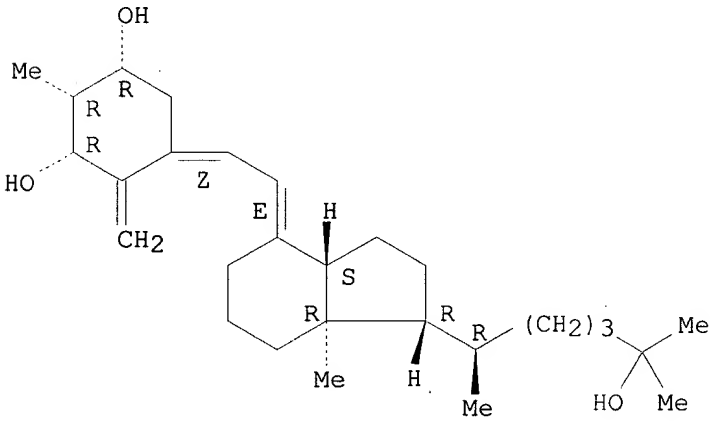

RN 203126-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



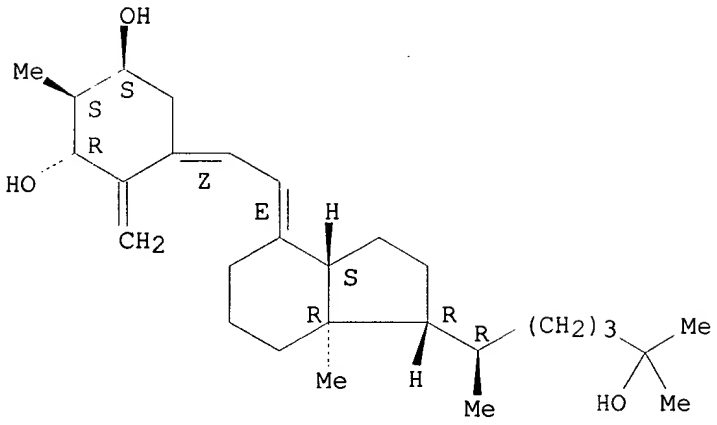

RN 203126-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



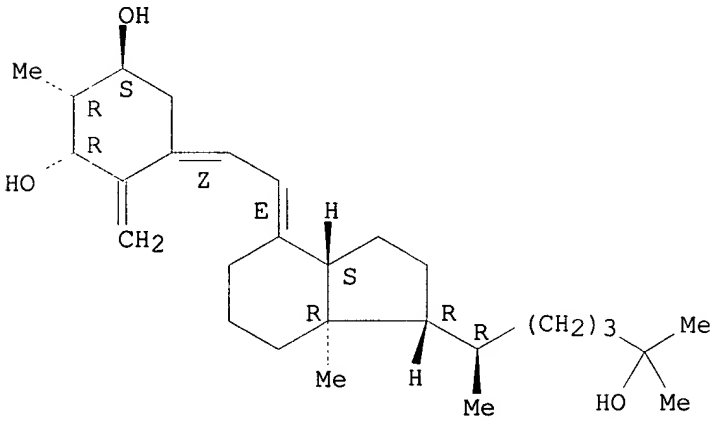

RN 203126-95-8 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

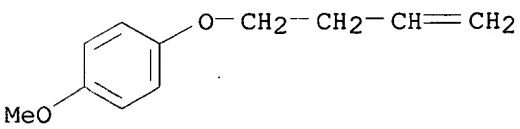


RN 203126-96-9 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.beta.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



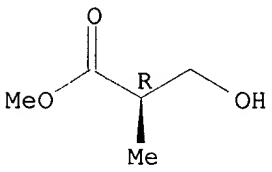
IT **2653-90-9 72657-23-9**, Methyl (R)-3-hydroxy-2-methylpropionate **80657-57-4**, Methyl (S)-3-hydroxy-2-methylpropionate **143705-63-9**
RL: RCT (Reactant)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)
RN 2653-90-9 HCAPLUS
CN Benzene, 1-(3-butenyloxy)-4-methoxy- (7CI, 9CI) (CA INDEX NAME)



RN 72657-23-9 HCAPLUS

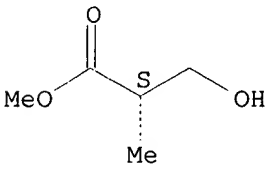
CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



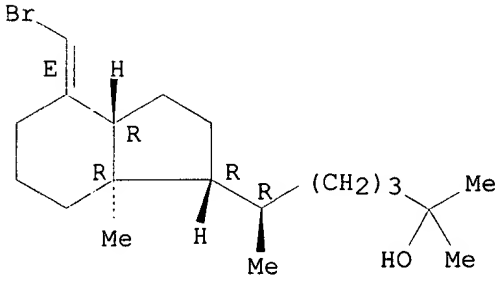

RN 80657-57-4 HCAPLUS
CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).




RN 143705-63-9 HCAPLUS
CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)-(9CI) (CA INDEX NAME)

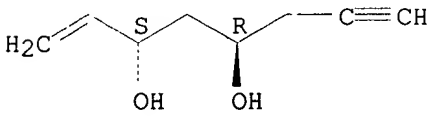
Absolute stereochemistry.
Double bond geometry as shown.




IT **152032-72-9P 161055-41-0P 169310-79-6P**
**169315-01-9P 203126-72-1P 203126-74-3P**
**203126-76-5P 203126-78-7P 203126-79-8P**
**203126-80-1P 203126-81-2P 203126-83-4P**
**203126-84-5P 203126-85-6P 203126-86-7P**
**203126-87-8P 203126-88-9P 203126-89-0P**
**203126-90-3P 203126-97-0P 203126-98-1P**
**203126-99-2P 203127-00-8P 203127-01-9P**
**203127-02-0P 203127-03-1P 203127-04-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)

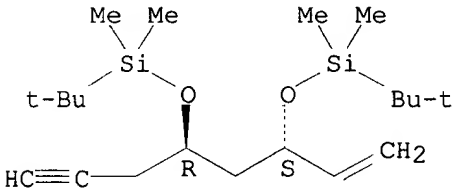
RN 152032-72-9 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



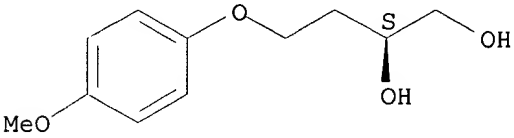
RN 161055-41-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane,
5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, (5S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



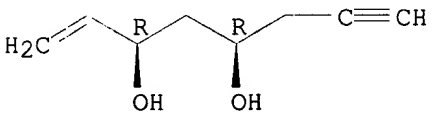
RN 169310-79-6 HCAPLUS
CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



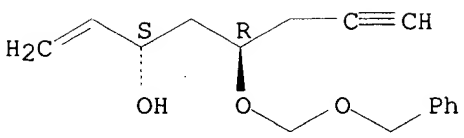
RN 169315-01-9 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



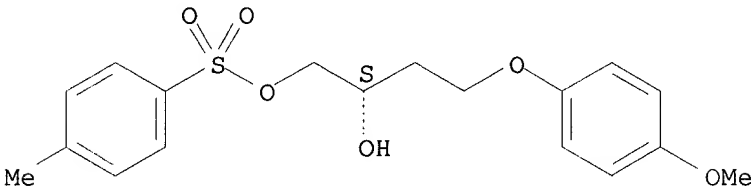
RN 203126-72-1 HCAPLUS
CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



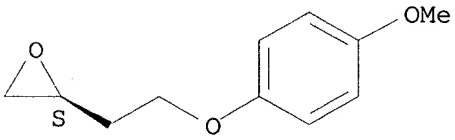
RN 203126-74-3 HCAPLUS
CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, 1-(4-methylbenzenesulfonate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



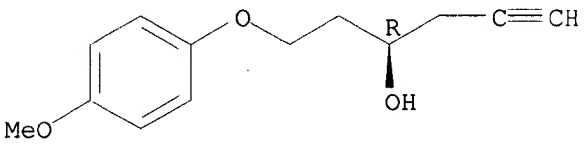
RN 203126-76-5 HCAPLUS
CN Oxirane, [2-(4-methoxyphenoxy)ethyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



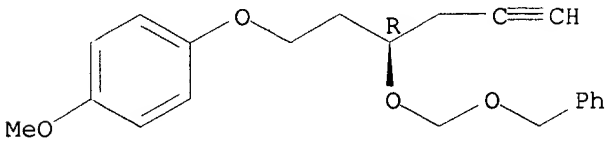
RN 203126-78-7 HCAPLUS
CN 5-Hexyn-3-ol, 1-(4-methoxyphenoxy)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



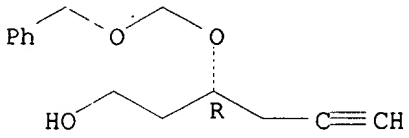
RN 203126-79-8 HCAPLUS
CN Benzene, 1-methoxy-4-[[3-[(phenylmethoxy)methoxy]-5-hexynyl]oxy]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



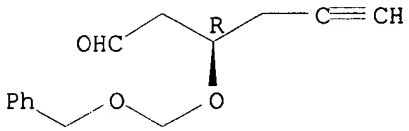
RN 203126-80-1 HCAPLUS
CN 5-Hexyn-1-ol, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



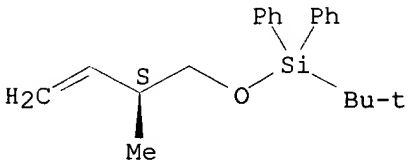

RN 203126-81-2 HCAPLUS
CN 5-Hexynal, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



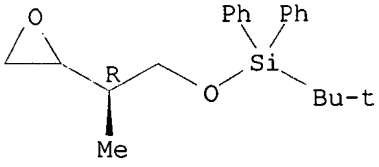

RN 203126-83-4 HCAPLUS
CN Silane, (1,1-dimethylethyl)[(2-methyl-3-butenyl)oxy]diphenyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



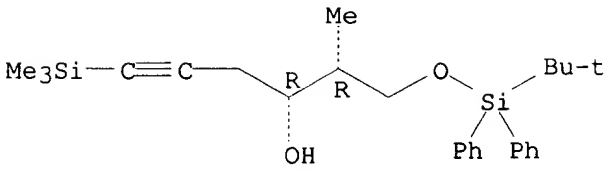

RN 203126-84-5 HCAPLUS
CN Silane, (1,1-dimethylethyl)(2-oxiranylpropoxy)diphenyl-, [2(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



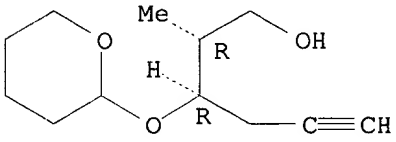

RN 203126-85-6 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



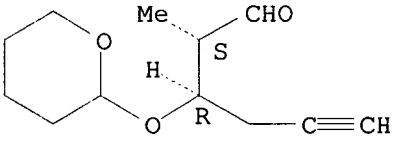
RN 203126-86-7 HCAPLUS
CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, [2(2R,3R)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



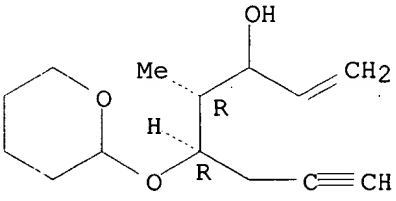
RN 203126-87-8 HCAPLUS
CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, [2(2S,3R)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



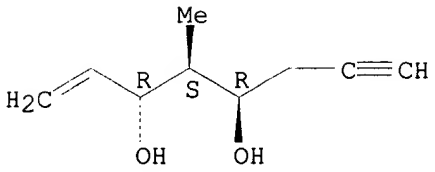
RN 203126-88-9 HCAPLUS
CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, [2(4R,5R)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



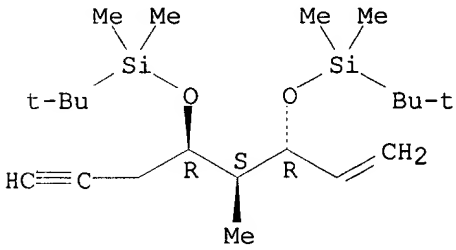
RN 203126-89-0 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, [3R-(3R*,4S*,5R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



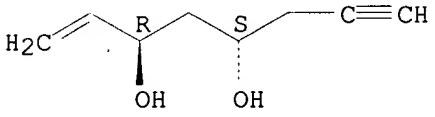
RN 203126-90-3 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



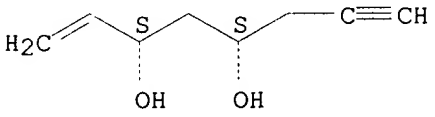
RN 203126-97-0 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



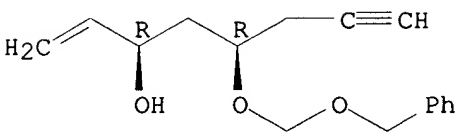
RN 203126-98-1 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



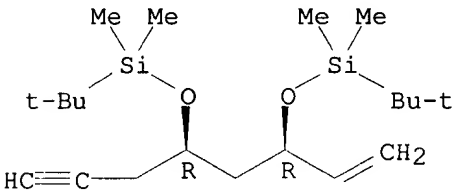
RN 203126-99-2 HCAPLUS
CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



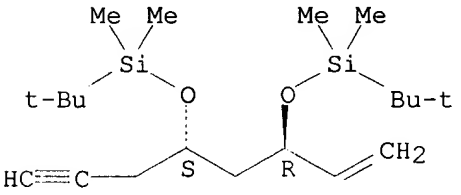
RN 203127-00-8 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



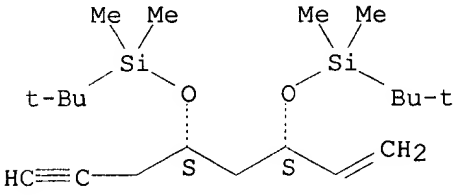
RN 203127-01-9 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



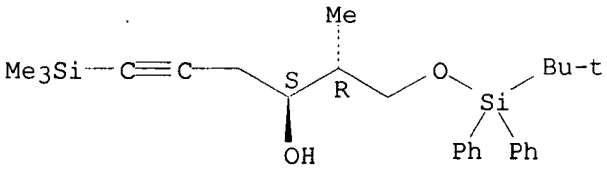
RN 203127-02-0 HCAPLUS
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-propynyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



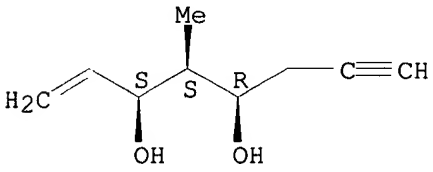
RN 203127-03-1 HCAPLUS
CN 5-Hexyn-3-ol, 1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



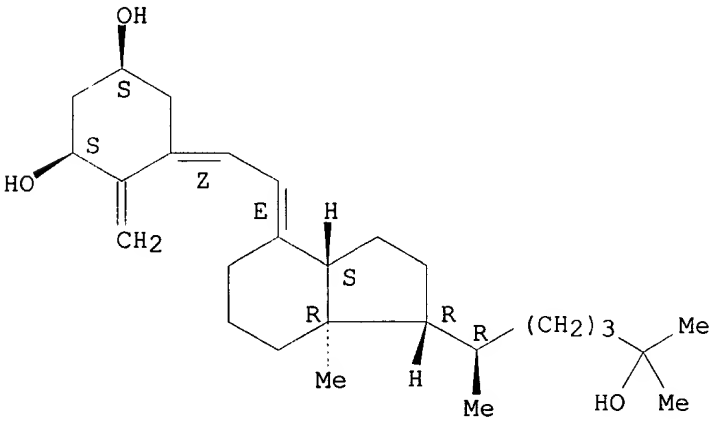
RN 203127-04-2 HCAPLUS
CN 1-Octen-7-yne-3,5-diol, 4-methyl-, [3S-(3R*,4R*,5S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **61476-45-7P 66791-71-7P 96614-28-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)
RN 61476-45-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

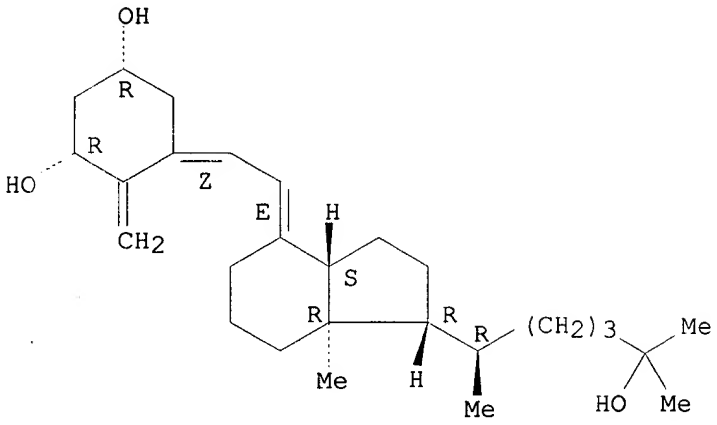
Absolute stereochemistry.
Double bond geometry as shown.



RN 66791-71-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.beta.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.




RN 96614-28-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.beta.,3.alpha.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.